Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
                 INSPEC enhanced with 1898-1968 archive
        AUG 09
NEWS
                ADISCTI Reloaded and Enhanced
        AUG 28
NEWS
        AUG 30
                CA(SM)/CAplus(SM) Austrian patent law changes
NEWS
        SEP 11
NEWS
                 CA/CAplus enhanced with more pre-1907 records
NEWS
        SEP 21
                 CA/CAplus fields enhanced with simultaneous left and right
                 truncation
NEWS
     8
        SEP 25
                 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS
     9
         SEP 25
                CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10
        SEP 25
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11
        SEP 28
                 CEABA-VTB classification code fields reloaded with new
                 classification scheme
NEWS 12 OCT 19
                LOGOFF HOLD duration extended to 120 minutes
NEWS 13 OCT 19
                E-mail format enhanced
NEWS 14 OCT 23
                Option to turn off MARPAT highlighting enhancements available
NEWS 15 OCT 23
                CAS Registry Number crossover limit increased to 300,000 in
                multiple databases
NEWS 16 OCT 23
                The Derwent World Patents Index suite of databases on STN
                 has been enhanced and reloaded
NEWS 17 OCT 30
                CHEMLIST enhanced with new search and display field
NEWS 18 NOV 03
                JAPIO enhanced with IPC 8 features and functionality
NEWS 19
        NOV 10
                CA/CAplus F-Term thesaurus enhanced
NEWS 20
        NOV 10
                STN Express with Discover! free maintenance release Version
                 8.01c now available
NEWS 21
        NOV 13
                CA/CAplus pre-1967 chemical substance index entries enhanced
                 with preparation role
        NOV 20
NEWS 22
                CAS Registry Number crossover limit increased to 300,000 in
                 additional databases
NEWS 23
        NOV 20
                CA/CAplus to MARPAT accession number crossover limit increased
                 to 50,000
NEWS 24
        NOV 20
                CA/CAplus patent kind codes will be updated
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
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              Welcome Banner and News Items
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              For general information regarding STN implementation of IPC 8
NEWS X25
              X.25 communication option no longer available
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 11:12:19 ON 30 NOV 2006

=>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:12:27 ON 30 NOV 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8 DICTIONARY FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

Uploading c:\documents and settings\pzucker\my documents\examination auxillary files\10025947\10025947 clm 1 amdt 8.9.06

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

T.1

STR

$$G_{2}$$
 G_{2}
 G_{3}
 G_{4}
 G_{2}
 G_{5}
 G_{6}

G1 CH2, O, S, N

G2 0, S

Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 11:13:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1308644 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

23 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 26115204 TO 26230556 PROJECTED ANSWERS: 293640 TO 308336

L2 23 SEA SSS SAM L1

=> d scan

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C21 H22 Br N O5

$$\begin{array}{c|c} O & \\ MeO-C & \\ \hline \\ CH_2-O-C-CH_2-CH_2-C-NH \\ \hline \\ Br & Me \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzeneethanimidamide, 4-nitro-N-(1-oxo-2-phenoxybutoxy)- (9CI)

MF C18 H19 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-[3-(phenylmethoxy)phenyl]-1-butenyl]-5-oxo-, (2R)- (9CI)

MF C28 H35 N O5

Absolute stereochemistry.

Double bond geometry as shown.

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C21 H24 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-[[2-[[(3,4-dimethylphenyl)amino]carbonyl]phenyl]amino]-4oxo- (9CI)

MF C19 H20 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanedioic acid, 3-[(E)-[[(1R,2R)-2-[(E)-[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-5-(1,1-dimethylethyl)-4-hydroxyphenyl methyl ester (9CI)

MF C38 H54 N2 O6

Absolute stereochemistry.

Double bond geometry as shown.

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Absolute stereochemistry.

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Crotonic acid, 3-[p-(methylpropylamino)anilino]-, ethyl ester (6CI)

MF C16 H24 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Aspartic acid, N-(4-methylphenyl)- (9CI)

MF C11 H13 N O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Thia-2,6-diazabicyclo[3.2.0]heptane-6-acetic acid, α -[3-[4-(chloromethyl)phenyl]-2-oxopropylidene]-2-[(1,1-dimethylethoxy)carbonyl]-3,3-dimethyl-7-oxo-, 1,1-dimethylethyl ester, [1R-[1 α ,5 α ,6(Z)]]- (9CI)

MF C27 H35 C1 N2 O6 S

Absolute stereochemistry.

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Heptenoic acid, 7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxy-5-(3-methoxyphenyl)-1-penten-4-ynyl]cyclopentyl]-, (5Z)- (9CI)

MF C24 H30 O6

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Histidinamide, N3,N5-bis[N3,N5-bis(N-acetyl-L-seryl)-3,5-diaminobenzoyl-L- α -aspartyl]-3,5-diaminobenzoyl-L-cysteinyl-, (5 \rightarrow 5'''')- disulfide with N3,N5-bis[N3,N5-bis(N-acetyl-L-histidyl)-3,5-diaminobenzoyl-L- α -aspartyl]-3,5-diaminobenzoyl-L-cysteinyl-L-serinamide (9CI)

SQL 22,6,6,3,3,1,1,1,1 MF C125 H146 N40 O43 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-B

_OH

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-oxo-4-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]-, ethyl ester (9CI)

MF C12 H17 N3 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Decanoic acid, 10-[[3,5-bis[1-[(aminoiminomethyl)hydrazono]ethyl]phenyl]am ino]-10-oxo-, dihydrochloride (9CI)

MF C22 H35 N9 O3 . 2 C1 H

●2 HCl

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 2-[[3-(2-methoxyphenyl)-4-oxo-4H-1-benzopyran-7-yl]oxy]-,
hexyl ester (9CI)

MF C26 H30 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN-

IN 3-Thiophenehexanoic acid, 2,5-dibromo- (9CI)

MF C10 H12 Br2 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Pyrazole-5-undecanoic acid, 1-methyl- (9CI)

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 3-Pentenoic acid, 5-(3-aminobicyclo[2.2.1]hept-2-yl)-, methyl ester, $[1\alpha, 2\alpha(Z), 3\beta, 4\alpha]$ -, trifluoroacetate (9CI) MF C13 H21 N O2 . C2 H F3 O2

CM 1

Relative stereochemistry.

Double bond geometry as shown.

CM 2

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 6-Octenoic acid, 8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5yl]-, [2α,4α,5α(Z)]-, compd. with 1,2-ethanediamine
(9CI)
MF C19 H23 F3 O5 . x C2 H8 N2

CM 1

Relative stereochemistry.

Double bond geometry as shown.

CM 2

 $H_2N-CH_2-CH_2-NH_2$

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C26 H43 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Lysine, N6-[2-(dithiocarboxy)-1-cyclopenten-1-yl]- (9CI)

MF C12 H20 N2 O2 S2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Heptenoic acid, $7-[2-[4-(3-\text{chlorophenoxy})-3-\text{hydroxy}-4-\text{methyl}-1-\text{pentenyl}]-3-\text{hydroxy}-5-\text{oxocyclopentyl}]-, methyl ester, [1R-[1<math>\alpha$ (Z),2 β (1E,3R*),3 α]]- (9CI)

MF C25 H33 C1 O6

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 12.32 12.53

FULL ESTIMATED COST

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 11:29:14 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

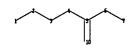
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 11:43:13 ON 30 NOV 2006 FILE 'REGISTRY' ENTERED AT 11:43:13 ON 30 NOV 2006 COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
12.32
12.53

=>

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By CI NE FIGURE



```
chain nodes :
1 2 3 4 5 6 7 10
chain bonds :
1-2 2-3 3-4 4-5 5-6 5-10 6-7
exact/norm bonds :
1-2 2-3 3-4 5-6 5-10 6-7
exact bonds :
4-5
G1:CH2,O,S,N
G2:0,S
Hydrogen count :
4:>= minimum 2
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 10:CLASS
Generic attributes :
3:
Type of chain
                     : Linear
Element Count :
```

Node 3: Limited C,C3-12

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

G1 CH2, O, S, N

G2 0, S

Structure attributes must be viewed using STN Express query preparation.

=> search 13 sss sam
SAMPLE SEARCH INITIATED 11:44:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1308644 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 9 ANSWERS

•

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

26115204 TO 26230556

PROJECTED ANSWERS:

113176 TO 122378

L4 9 SEA SSS SAM L3

=> d scan

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 2-[[3-(2-methoxyphenyl)-4-oxo-4H-1-benzopyran-7-yl]oxy]-, hexyl ester (9CI)

MF C26 H30 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Octenoic acid, $8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5-yl]-, [2<math>\alpha$, 4α , 5α (Z)]-, compd. with 1,2-ethanediamine (9CI)

MF C19 H23 F3 O5 . x C2 H8 N2

CM 1

Relative stereochemistry.

Double bond geometry as shown.

CM 2

H2N-CH2-CH2-NH2

IN

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

3-Thiophenehexanoic acid, 2,5-dibromo- (9CI)

MF C10 H12 Br2 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-oxo-4-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]-, ethyl ester (9CI)

MF C12 H17 N3 O5

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 1H-Pyrazole-5-undecanoic acid, 1-methyl- (9CI) MF C15 H26 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1,3-Dioxolane-4-heptanoic acid, 5-[1-hydroxy-3-[4[(trimethylsilyl)ethynyl]phenyl]-2-propynyl]-2-oxo-, methyl ester,
[4S-[4α,5β(R*)]]- (9CI)
MF C25 H32 O6 Si

Absolute stereochemistry.

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Hexanoic acid, 6-[(1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy]-, methyl ester (9CI)

MF C21 H24 N2 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Nonanoic acid, 9-[(2-0- α -D-mannopyranosyl- α -D-

mannopyranosyl)oxy]-, methyl ester (9CI)

MF .C22 H40 O13

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e Hexanoic acid, 6-[(1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy]-/cn

E1	1	HEVANOTO AGID (7 DIMHIADICUCIO/2 0 1) OGM 0 VI DOMED G OVI		
FI	1	HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER, S-OXI DE, (ENDO, ANTI)-/CN		
E2	1	HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER, S-OXI		
E3	0>	DE, (EXO,ANTI)-/CN HEXANOIC ACID, 6-(1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OX Y-/CN		
E4	1	HEXANOIC ACID, 6-((((((((3,4-DICHLOROPHENYL)METHYL)AMINO)IMIN		
E 5	1	OMETHYL) AMINO) IMINOMETHYL) AMINO) -/CN HEXANOIC ACID, 6-(((((2-(((3,5-BIS(1,1-DIMETHYLETHYL)-2-HYD ROXYPHENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) P		
E6	1	HENYLACETYL) AMINO) -, (1R-(1A(S*),2B))-/CN HEXANOIC ACID, 6-(((((2-(((3,5-DIBROMO-2-HYDROXYPHENYL) METH YLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYLACETYL) AMI NO)-, (1R-(1A(S*),2B))-/CN		
E7 ·	1	HEXANOIC ACID, 6-((((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-5-METHOXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN		
E8	1	HEXANOIC ACID, 6-(((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-5-NITROPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMIN		
E9	1	O) PHENYLACETYL) AMINO) -, (1R-(1A(S*), 2B)) -/CN HEXANOIC ACID, 6-(((((2-(((3-(1,1-DIMETHYLETHYL)-2-HYDROXYP HENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYL		
E10	1	ACETYL) AMINO) -, (1R-(1A(S*),2B))-/CN HEXANOIC ACID, 6-(((((2-(((5-(1,1-DIMETHYLETHYL)-2-HYDROXYP HENYL) METHYLENE) AMINO) CYCLOHEXYL) AMINO) CARBONYL) AMINO) PHENYL		
E11	1 .	ACETYL) AMINO) -, (1R-(1A(S*),2B))-/CN HEXANOIC ACID, 6-(((((2-((2-((1-NAPHTHALENYLCARBONYL) AMINO) -1-OXO-3-(1-(TRIPHENYLMETHYL)-1H-IMIDAZOL-4-YL) PROPYL) AMINO) CYCLOHEYYL OYYL CARRONYL AMINO ACEMYL AMINO (12 (14		
E12	1	CYCLOHEXYL) OXY) CARBONYL) AMINO) ACETYL) AMINO) -, (1S-(1A, 2B(R*))) -/CN HEXANOIC ACID, 6-(((((4-ETHOXYPHENYL) AMINO) CARBONYL) AMINO) O XOACETYL) AMINO) -/CN		
		l, 6-((1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy)-/cn		
E1 E2	1 1	HEXANOIC ACID, 6-((1-IMINOETHYL)AMINO)-2-OXO-/CN HEXANOIC ACID, 6-((1-METHOXY-2-NITROETHENYL)AMINO)-, METHYL		
E3	0>	ESTER/CN HEXANOIC ACID, 6-((1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OX		
E4	1	Y)-/CN HEXANOIC ACID, 6-((1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OX		
E5	1	Y)-, METHYL ESTER/CN HEXANOIC ACID, 6-((1-METHYL-3-(2-((2-METHYL-1-OXO-2-PROPENYL		
	*)OXY)ETHOXY)-3-OXO-1-PROPENYL)AMINO)-/CN		
E6	1	HEXANOIC ACID, 6-((1-METHYL-3-OXO-1-BUTENYL)OXY)-, ETHYL EST ER/CN		
E7	1	HEXANOIC ACID, 6-((1-METHYL-5-NITRO-1H-IMIDAZOL-2-YL)THIO)-/CN		
E8	1	HEXANOIC ACID, 6-((1-METHYLCYCLOHEXADECYL)OXY)-/CN		
E9	1	HEXANOIC ACID, 6-((1-METHYLCYCLOHEXADECYL)OXY)-, METHYL ESTE R/CN		
E10	1	HEXANOIC ACID, 6-((1-METHYLETHOXY)AMINO)-4,6-DIOXO-/CN		
E11	1	HEXANOIC ACID, 6-((1-METHYLETHYL)(3-METHYL-5-(2-(4-PYRIDINYL AMINO)ETHOXY)BENZOYL)AMINO)-/CN		
E12	1	HEXANOIC ACID, 6-((1-METHYLETHYL) (3-METHYL-5-(2-(4-PYRIDINYL AMINO)ETHOXY)BENZOYL)AMINO)-, MONO(TRIFLUOROACETATE)/CN		
=> d cost				
COST IN U.S.	. DOLLA	RS SINCE FILE TOTAL ENTRY SESSION		
CONNECT CHAI	RGES	13.30 13.45		
NETWORK CHAI		2.10 2.16		

=> logoff hold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 15.40 15.61

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 11:47:31 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 12:22:51 ON 30 NOV 2006 FILE 'REGISTRY' ENTERED AT 12:22:51 ON 30 NOV 2006 COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.40	15.61
-> logoff hold		

=> logoff hold
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
15.40
15.61

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 12:23:04 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 12:47:30 ON 30 NOV 2006 FILE 'REGISTRY' ENTERED AT 12:47:30 ON 30 NOV 2006 COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	15.40	15.61

=> e 4-phenyl-2-butynoic acid/cn E1 1 4-PHENYL-2-BUTYN-1-OL/CN

E2 1 4-PHENYL-2-BUTYN-1-YL CHRYSANTHEMATE/CN

E3 1 --> 4-PHENYL-2-BUTYNOIC ACID/CN E4 1 4-PHENYL-2-CHLOROPHENOL/CN

```
E5
                   4-PHENYL-2-CYANOCYCLOBUTANONE/CN
E6
                   4-PHENYL-2-CYANOPYRIDINE/CN
E7
             1
                   4-PHENYL-2-CYCLOHEXEN-1-ONE/CN
E8
             1
                   4-PHENYL-2-CYCLOPENTEN-1-ONE/CN
E9
             1
                   4-PHENYL-2-CYCLOPENTENONE/CN
E10
            1
                   4-PHENYL-2-ETHOXY-N-(2-(3-METHOXY-4-((2-PROPYNYL)OXY)PHENYL)
                   ETHYL) PENTANAMIDE/CN
E11
                   4-PHENYL-2-ETHOXYOXETANE/CN
E12
                   4-PHENYL-2-FLAVENE/CN
=> e3
L5
             1 "4-PHENYL-2-BUTYNOIC ACID"/CN
=> d 15
L5
    ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN
     40886-84-8 REGISTRY
     Entered STN: 16 Nov 1984
CN 2-Butynoic acid, 4-phenyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
    Tetrolic acid, phenyl- (7CI)
OTHER NAMES:
     4-Phenyl-2-butynoic acid
CN
MF
     C10 H8 O2
                 BEILSTEIN*, CA, CAOLD, CAPLUS
LC
     STN Files:
         (*File contains numerically searchable property data)
```

 $HO_2C-C \equiv C-CH_2-Ph$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> 105

L6 8 LO5

=> 15

L7 3 L5

=> d 17 1-3 ti fbib abs

- L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Acetylenic acids. I. Reaction of arylpropiolic acids with carbodiimides
- AN 1973:147497 CAPLUS
- DN 78:147497
- TI Acetylenic acids. I. Reaction of arylpropiolic acids with carbodiimides
- AU Cadby, P. A.; Hearn, M. T. W.; Ward, A. D.
- CS Org. Chem. Dep., Univ. Adelaide, Adelaide, Australia
- SO Australian Journal of Chemistry (1973), 26(3), 557-70 CODEN: AJCHAS; ISSN: 0004-9425
- DT Journal
- LA English
- AB The formation of substituted 1-phenynaphthalene-2,3-dicarboxylic anhydrides from substituted phenylpropiolic acids by carbodimides is a general reaction and proceeds in high yields under mild conditions. Heterocyclic acetylenic acids also form analogous products in high yield The reaction is comfined to α,β -acetylenic acids conjugated with an aromatic ring, as alkyl-propiolic acids form mixts. of alkylpropiolic anhydrides and N-acylureas under the same conditions and esters of arylpropiolic acids do not react. The effects of temperature, bases, and solvents on the reaction are described. Some features of the NMR spectra of the 1-phenylnaphthalene products are discussed.
- L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI A model for the natural synthesis of allenes
- AN 1964:2723 CAPLUS
- DN 60:2723
- OREF 60:402g-h
- TI A model for the natural synthesis of allenes
- AU Cymerman-Craig, J.; Moyle, M.
- CS Univ. California, San Francisco
- SO Journal of the Chemical Society (1963), (Nov.), 5356-60 CODEN: JCSOA9; ISSN: 0368-1769
- DT Journal
- LA Unavailable
- OS CASREACT 60:2723
- AB The closest available model for a β -polyketone, acetonedicarboxylic ester, was transformed into dimethyl penta-2,3-dienedioate through its enol phosphate which was decomposed by aqueous alkali in 10 sec. at 0°. The enol phosphate of γ -phenylacetoacetic ester needed 24 hrs. for complete elimination. The reaction requires activation in both the groups R and R' in RCH2COCH2R', in a manner similar to that in natural β -polyketones. A possible mechanism for the concurrent formation of acetylenes and allenes in nature is proposed.
- L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Addition reactions of acetylenes. I. Chloroformylation of arylacetylenic compds
- AN 1963:428242 CAPLUS
- DN 59:28242
- OREF 59:5043c-h,5044a-d

```
TI
     Addition reactions of acetylenes. I. Chloroformylation of arylacetylenic
AU
     Yen, Vo-Quang
SO
     Ann. Chim. (Paris) (1962), 7, 785-99
DΤ
     Journal
LА
     Unavailable
OS
     CASREACT 59:28242
     PhCOMe (0.1 mole) added in small portions to 0.1 mole cold PC15 and the
AΒ
     mixture heated 0.5 hr. at 70-80° gave 64% \alpha-chlorostyrene. The
     p-bromo- (b13 122-5°), p-methyl- (I), and p-methoxy-\alpha-
     chlorostyrenes were similarly prepared from p-bromo-, p-methyl-,
     p-methoxyacetophenone in 77, 74.5, and 35% yields, resp.
     Dehydrohalogenation of I by treatment with NaNH2 in liquid NH3 overnight
     gave 61% p-MeC6H4C:CH; this was a much higher yield than was obtained when
     the reaction was carried out with KOH in alc. at 100°, or with
     NaNH2 at 150°. PhC:CH (0.5 mole) refluxed 1 hr. with 0.5 mole Na in
     400 ml. anhydrous tetrahydrofuran (THF), 0.5 mole Me2SO4 added slowly, and
     the mixture refluxed 1 hr. gave 47% 1 phenyl-1-propyne (II).
     1-(p-Tolyl)-1-propyne (III) (b1 70°), and 1-[p-anisyl)-1-propyne
     (IV) were similarly prepared from p-tolylacetylene and p-anisylacetylene in
     49 and 41% yields, resp. Propargyl bromide (0.5 mole) added slowly to a
     cold Et2O solution of PhMgBr from 0.5 mole PhBr, and the solution refluxed 1
hr.
     gave 65.5% mixture of II, 1-phenylallene, and 1-phenyl2-propyne; 11.6 g. of
     this mixture gave 82% yield of II (95.5% pure) on isomerization by boiling
     10 min. with 1 g. KOH in 50 ml. dry THF. III and IV were similarly
     obtained from p-bromotoluene and p-bromoanisole in 70 and 52% yields for
     the 1st step, and 80 (92.6% pure) and 75% (93.4% pure) yields for the
     isomerization, resp.; the isomerizations in these eases were carried out
     for 1 hr. The isomerization reactions ArCH2C:CH .dblharw. ArCH:C:CH2
     .dblharw. ArC:CMe, where Ar = Ph, p-MeC6H4, or p-MeOC6H4, were studied by
     gas chromatography, infrared and Raman spectroscopy, and by determination of
     acetylenic bonds. The yields of the 1-aryl-1-propynes decreased if the
     isomerization time was increased, probably because of polymerization of
     the intermediate arylallenes. The mechanism of chloroformylation is
     discussed. A study of chloroformylation showed: (1) the presence of a
     solvent or an increase in temperature at the beginning of the reaction
decreased
     the yield; (2) the best yields were obtained at .apprx.0° and a
     reaction time of 10 hrs.; (3) stirring increased the yield. HCONMe2 could
     not replace N-methylformanilide (V) in chloroformylation of PhC:CH; excess
     POC13 increased the yield; excess V had no influence. The general
     procedure for formylation of \alpha-chlorostyrenes and for
     chloroformylation of arylacetylenes consisted in stirring, 0.5 hr. at
     0°, a mixture of 0.1 mole V and 0.12 mole POCl3, adding slowly 0.1
     mole of the compound to be formylated or chloroformylated, and then
     continuing to stir 15 hrs. at 0°. The following ArCCl: CHCHO were
     prepared [Ar, yield when prepared from ArC:CH, yield when prepared from
     ArCCl:CH2, and (if new compds.) m.p. or b.p., and m.ps. of semicarbazone,
     phenylhydrazone, 2,4dinitrophenylhydrazone, and oxime given]: Ph, 39%,
     45%, -, 234°, 150°, 226°, 78°; p-BrC6H4, 41%,
     24%, 102°, 233°, 157°, 258°, 120°;
     p-MeC6H4, 46%, 68%, b0.5 120°, 256°, 148°
     235°, 110°; and p-MeOC6H4, 67%, 51%, -, 225°, 158°, 210°, 137°. Tire following ArCCl: CMeCHO were
     prepared from the corresponding ArC:CMe (Ar, % yield, b.p., and m.ps. of
     semicarbazone, 2,4-dinitrophenylhydrazone, and oxime given): Ph, 47%, b0.5 94°, 162° (155°), 227° (155°), 120°; p-MeC6H4, 53.5%, b0.5 102°, 228°, 196° (210°), 155°; and p-MeOC6H6, 55%, b0.5
```

p-Diethynylbenzene gave 20% 1-chloro-1-p-ethynylphenylpropen-3-al; semicarbazone m. 260° (decomposition); 2,4-dinitrophenylhydrazone m.

135° (m. 44°), 250°, 184°, 126°.

245°; 9,10-diethynylanthracene gave 17.5% 9,10-bis(1-chloropropen-3al)anthracene, m. 215°. The liquid chlorinated aldehydes decomposed slowly in air and light. Oxidation of the arylchloropropenals (0.01 mole) was carried out in aqueous-alc. solution by stirring overnight with 0.04 mole AgNO3 and 0.08 mole NaOH. The following Arccl: CRCO2H were formed [Ar, R, % yield, and m.p. (if a new compound) given]: Ph, H, 56%, -; p-BrC6H4, H, 68, 173°; p-MeC6H4, H, 61, 168°; p-MeOC6H4, H, 47, 166°; Ph, Me, 58, -; and p-MeC6H4, Me, 43, 107°. For purposes of comparison with these acids, ArCHo2CCMgBr was treated overnight with dry ice and the α -acetylenic acids obtained were treated with a current of dry HCl at 90-100° for 5-10 hrs.; the following ArCH2C:CCO2H (VI) and ARCH2CCl:CHCO2H (VII) were obtained far, % yield of VI, m.p. of VI, % yield of VII, and m.p. of VII given): Ph, 34.5, 48°, 41, 90°; p-MeC6H4, 35, 72°, 47.5, 94°; and p-MeOC6H4, 31, 86°, 43, 80°. The infrared spectra of VI and VII were compared. The arylchloropropenals (0.001 mole in the case of condensation with an atiphatic ketone, or 0.002 mole with a cyclic ketone) and 0.001 mole ketone were dissolved in 10 ml. EtOH, the mixture was heated to 50°, a few drops of fresh 5% aqueous NaOH solution added, and the mixture kept at 51° .apprx.10 min.; the following chalcones were thus prepared: Arccl:CRCH:CHCOAr' (Ar, R, Ar', % yield, and m.p. given): Ph, H, Ph, 52, 90°; Ph, H, p-BrC6H4, 61, 130°; Ph, H, p-ClC6H4, 60, 124°; Ph, H, p-MeOC6H4, 69, 134°; p-MeC6H4, H, Ph, 49, 75°; p-MeC6H4, H, p-BrC6H4, 57, 148°; p-MeC6H4, H, p-ClC6H4, 62, 143°; p-MeC6H4, H, p-MeC6H4, 54, 99°; Ph, Me, Ph, 62, 110°; Ph, Me, p-McC6H4, 57, 95°; Ph, Me, p-MeC6H4, 63, 124°; p-MeC6H4, Me, p-BrC6H4, 51, 113°; p-MeC6H4, Me, p-ClC6H4, 55, 117°; p-MeC6H4, Me, p-MeC6H4, 59, 100°; and p-MeC6H4, Me, p-MeC6H4, 66, 143°. VIIa (ar, R, % yield, and m.p. given): Ph, H, 72, 165°; p-MeC6H4, H, 69, 194°; p-MeC6H4, H, 76, 195°; Ph, Me, 68, 186°; and p-MeC6H4, Me, 64, 180°; and VIIb (Ar, R, % yield, and m.p. given): Ph, H, 71, 216°; p-MeC6H4, H, 74, 244°; p-MeOC6H4, H, 75, 180°; Ph, Me, 67, 143°; and p-MeC6H4, Me, 61, 149°. The ultraviolet spectra of the chalcones were determined V and POC13 with phenylallene gave 2-chloromethyl-1-phenylpropen-3-al, m. 67°, whose ultraviolet and nuclear magnetic resonance spectra were determined

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=> e 5-tetrahydropyranyloxy-2-pentenoic acid/cn				
E1	1	5-TETRAHYDROFURFURYLOXY-4-OXO-4H-1-BENZOPYRAN-2-CARBOXAMIDE/		
		CN		
E2	1	5-TETRAHYDROPTEROYLTRIGLUTAMATE METHYLTRANSFERASE/CN		
E3	0>	5-TETRAHYDROPYRANYLOXY-2-PENTENOIC ACID/CN		
E4	1	5-TETRAHYDROPYRANYLOXY-7-BENZOFURANCARBOXALDEHYDE/CN		
E5	1	5-TETRALINCARBOXALDEHYDE/CN		
E6	1	5-TETRALINYLAMINE/CN		
E7	1	5-TETRAPHOSPHABOROLANAMINE, 1,2,3,4-TETRAKIS(1,1-DIMETHYLETH		
		YL)-N,N-BIS(1-METHYLETHYL)-, (1A,2B,3A,4.BE		
		TA.)-/CN		
E8	1	5-TETRAPHTHENEMERCAPTAN/CN		
E9	1	5-TETRAPHTHENESULFINIC ACID/CN		
E10	1	5-TETRAPHTHENESULFONAMIDE/CN		
E11	_ 1	5-TETRAPHTHENESULFONANILIDE/CN		
E12	1	5-TETRAPHTHENESULFONIC ACID/CN		
•				

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L8 STRUCTURE UPLOADED

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L8 HAS NO ANSWERS

L8 STF

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SAMPLE SEARCH INITIATED 13:15:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 869 TO ITERATE

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869 ITERATIONS

34 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

15612 TO 19148

PROJECTED ANSWERS: 331 TO

L9

34 SEA SSS SAM L8

=> d scan

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Galactonic acid, 6-0- α -D-galactopyranosyl- (9CI)

MF C12 H22 O12

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glutamic acid, N-(3-hydroxy-1-oxotetradecyl)-, 5-[2-deoxy-3-O-(3-hydroxy-1-oxotetradecyl)-2-[(3-hydroxy-1-oxotetradecyl)amino]- α -D-glucopyranosyl] ester, [1(R),2(R),3(R)]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI)

MF C53 H98 N2 O14 . C4 H11 N O3

CM 1

PAGE 1-A

PAGE 1-B

$$-(CH2)10-Me$$

CM 2

$$\begin{array}{c} ^{\rm NH_2} \\ | \\ {\rm HO-CH_2-C-CH_2-OH} \\ | \\ {\rm CH_2-OH} \end{array}$$

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Gentiobionic acid, Ca salt (6CI)

MF C12 H22 O12 . 1/2 Ca

Absolute stereochemistry.

●1/2 Ca

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-manno-2-Octulosonic acid, O-2-(acetylamino)-2-deoxy-α-Dglucopyranosyl-(1→2)-O-3,7-bis-O-[(2-aminoethoxy)hydroxyphosphinyl]L-glycero-α-D-manno-heptopyranosyl-(1→3)-O-[β-Dglucopyranosyl-(1→4)]-O-L-glycero-α-D-manno-heptopyranosyl(1→5)-3-deoxy- (9CI)

MF C40 H73 N3 O36 P2

Absolute stereochemistry.

PAGE 2-A

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN L-Lysine, N2,N6-bis[(1,1-dimethylethoxy)carbonyl]-5-(β-D-galactopyranosyloxy)-, (5R)- (9CI)
MF C22 H40 N2 O12

Absolute stereochemistry. Rotation (-).

HO

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Lysine, 5-[(2-O- α -D-glucopyranosyl- β -D-galactopyranosyl)oxy]-, threo-(9CI)

MF C18 H34 N2 O13

CI COM

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 13,16-Docosadienoic acid, 2-hexyl-3-hydroxy-5-[(tetrahydro-2H-pyran-2-yl)oxy]- (9CI)

MF C33 H60 O5

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-N-acetyl- (9CI)

MF C33 H53 N3 O25

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

D-manno-2-Octulosonic acid, O-L-glycero-α-D-manno-heptopyranosyl(1→2)-O-D-glycero-α-D-manno-heptopyranosyl- (1→2)-Oα-D-galactopyranuronosyl- (1→3)-O-[L-glycero-α-D-manno-heptopyranosyl- (1→7)]-O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-Lglycero-α-D-manno-heptopyranosyl- (1→3)-O-[β-Dglucopyranosyl- (1→4)]-O-L-glycero-α-D-manno-heptopyranosyl(1→5)-O-[4-amino-4-deoxy-β-L-arabinopyranosyl- (1→8)]-3deoxy- (9CI)

MF C62 H107 N2 O55 P

Absolute stereochemistry.

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN D-manno-2-Octulosonic acid, $O-\alpha-D$ -galactopyranosyl- $(1\rightarrow6)-O$ - $[O-D-galactopyranosyl-(1\rightarrow4)-O-2-(acetylamino)-2-deoxy-D-glucopyranosyl-<math>(1\rightarrow3)-O-D$ -galactopyranosyl- $(1\rightarrow3)-O-2-(acetylamino)-2-deoxy-D-glucopyranosyl-<math>(1\rightarrow7)-O-L$ -glycero- α -D-manno-heptopyranosyl- $(1\rightarrow6)-O-\alpha$ -D-glucopyranosyl- $(1\rightarrow2)-\alpha$ -D-glucopyranosyl- $(1\rightarrow3)$]- $O-\alpha$ -D-glucopyranosyl- $(1\rightarrow3)$ - $O-[L-glycero-\alpha-D-manno-heptopyranosyl-<math>(1\rightarrow3)$ -O-L-glycero- α -D-manno-heptopyranosyl- $(1\rightarrow3)$ -O-L-glycero- α -D-manno-heptopyranosyl- $(1\rightarrow3)$ -O-L-glycero- α -D-manno-heptopyranosyl- $(1\rightarrow5)$ -3-deoxy-(9CI)

Absolute stereochemistry. Currently available stereo shown.

PAGE 1-A

PAGE 1-B

PAGE 2-B

PAGE 3-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Thiazoleacetic acid, $2-[[(1,1-dimethylethoxy)carbonyl]amino]-\alpha-[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbonyl]amino[3-(3-dimethylethoxy)carbo$

[(tetrahydro-2H-pyran-2-yl)oxy]propylidene]-, (E)- (9CI)

MF C18 H26 N2 O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2+8)-O-(N-acetyl- α -neuraminosyl)-(2+8)-N-acetyl-(9CI)

MF C110 H172 N10 081

PAGE 1-D

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Pentenoic acid, 3-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (Z)- (9CI)
MF C11 H18 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN L-erythro-L-gluco-Deconic acid, O-3-O-acetyl-2,6-dideoxy-3-C-methyl-4-O-(1-

oxopropyl)- α -L-ribo-hexopyranosyl- $(1\rightarrow 4)$ -O-2-O-acetyl-3,6-dideoxy-3-(dimethylamino)- β -D-glucopyranosyl- $(1\rightarrow 5)$ -10-[(4-azidobutyl)(4-phenylbutyl)amino]-2,6,7,8,10-pentadeoxy-6-(2,2-dimethoxyethyl)-8-methyl-4-O-methyl-, 9-acetate 3-propanoate (9CI) MF C57 H93 N5 O19

Absolute stereochemistry. Rotation (-).

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN Hexanoic acid, $6-[[O-(N-acetyl-\alpha-neuraminosyl)-(2\rightarrow3)-O-\beta-D-galactopyranosyl-(1\rightarrow4)-O-[6-deoxy-\alpha-L-galactopyranosyl-(1\rightarrow3)]-2-amino-2-deoxy-<math>\beta$ -D-glucopyranosyl]oxy]- (9CI)

MF C35 H60 N2 O24

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-manno-2-Octulosonic acid, O-[O-acetyl-2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-(1→2)-O-[α-D-glucopyranosyl-(1→3)]-O-L-glycero-α-D-manno-heptopyranosyl-(1→3)-O-[O-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-β-D-glucopyranosyl-(1→3)-O-β-D-galactopyranosyl-(1→4)-O-β-D-glucopyranosyl-(1→4)-β-D-glucopyranosyl-(1→4)]-O-L-glycero-α-D-manno-heptopyranosyl-(1→5)-3-deoxy-(9CI)

MF C70 H116 N2 O56

CI IDS
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CM 1

PAGE 1-A

PAGE 3-A

CM 2

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2+8)-O-(N-acetyl- α -neuraminosyl)-(2+8)-N-acetyl-(9CI) MF C132 H206 N12 O97

PAGE 1-B

PAGE 1-C

PAGE 1-D

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Neuraminic acid, N-(hydroxyacetyl)-8-O-[N-(hydroxyacetyl)- α -neuraminosyl]- (9CI)

MF C22 H36 N2 O19

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-erythro-L-gluco-Deconic acid, O-3-O-acetyl-2,6-dideoxy-3-C-methyl-4-O-(1-oxopropyl)-α-L-ribo-hexopyranosyl-(1→4)-O-2-O-acetyl-3,6-dideoxy-3-(dimethylamino)-β-D-glucopyranosyl-(1→5)-10-[(3-aminobutyl)(4-phenylbutyl)amino]-2,6,7,8,10-pentadeoxy-6-(2,2-dimethoxyethyl)-8-methyl-4-O-methyl-, 9-acetate 3-propanoate (9CI)
MF C57 H95 N3 O19

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,7-Octadienoic acid, 6-[(6-deoxy- β -D-glucopyranosyl)oxy]-2,6-dimethyl-, (2E,6R)- (9CI)

MF C16 H26 O7

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Octanoic acid, 8-chloro-6-[(tetrahydro-2H-pyran-2-yl)oxy]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI)

MF C13 H23 C1 O4 . C12 H23 N

CM 1

CM 2

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Nonenoic acid, 4-oxo-8-[(tetrahydro-2H-pyran-2-yl)oxy]-, (E)- (9CI)

MF C14 H22 O5

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Glutamic acid, N-acetyl-, $5-\alpha$ -D-glucopyranosyl ester (9CI)

MF C13 H21 N O10

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-manno-2-Octulosonic acid, O-[N-(4-aminobutyl)- β -D-galactopyranuronamidosyl]-(1 \rightarrow 7)-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 7)-O-[O-2-amino-2-deoxy- α -D-galactopyranosyl-(1 \rightarrow 4)- α -D-galactopyranuronosyl-(1 \rightarrow 3)]-O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-[β -D-glucopyranosyl-(1 \rightarrow 4)]-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 5)-O-[4-amino-4-deoxy- β -L-arabinopyranosyl-(1 \rightarrow 8)]-3-deoxy-(9CI)

Absolute stereochemistry.

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Propanedioic acid, $[3-(\beta-D-mannopyranosyloxy)-2-(octadecyloxy)propyl]-(9CI)$

MF C30 H56 O11

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN Neuraminic acid. O-[N-(1-oxopropyl)-α-neuraminosy

IN Neuraminic acid, O-[N-(1-oxopropyl)- α -neuraminosyl]-(2-8)-O-[N-(1-oxopropyl)- α -neuraminosyl]-(2-8)-O-[N-(1-oxopropyl)- α -neuraminosyl]-(2-8)-O-[N-(1-oxopropyl)- α -neuraminosyl]-(2-8)-O-[N-(1-oxopropyl)- α -neuraminosyl]-(2-8)-N-(1-oxopropyl)- (9CI)

MF C72 H116 N6 O49

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN D-manno-2-Octulosonic acid, O-2-(acetylamino)-2-deoxy- α -Laltropyranuronosyl-(1→3)-O-2-(acetylamino)-4-amino-2,4,6-trideoxy- β -D-galactopyranosyl-(1 \rightarrow 3)-O- β -D-glucopyranosyl- $(1\rightarrow 3)$ -O- $[O-\alpha-D-galactopyranosyl-<math>(1\rightarrow 2)$ - $\alpha-D$ galactopyranosyl- $(1\rightarrow2)$]-O- α -D-glucopyranosyl- $(1\rightarrow3)$ -O- α -D-glucopyranosyl-(1 \rightarrow 3)-O-[O-2-amino-2-deoxy- α -Dglucopyranosyl- $(1\rightarrow7)$ -L-glycero- α -D-manno-heptopyranosyl- $(1\rightarrow7)$]-O-L-glycero- α -D-manno-heptopyranosyl- $(1\rightarrow3)$ -O-4-O-(6-amino-1,3-dihydroxy-1,3-dioxido-2,4-dioxa-1,3-diphosphahex-1-y1)-Lglycero- α -D-manno-heptopyranosyl- $(1\rightarrow 5)$ -3-deoxy-(9CI)MF C83 H143 N5 O70 P2

PAGE 1-A

 $- cH_2 - NH_2$

$$H_2N$$
 OH CH_2-OH OH CH_2-OH

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Hexanoic acid, 6-[(tetrahydro-2H-pyran-2-yl)oxy]- (8CI, 9CI)

MF C11 H20 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Hexanoic acid, $6-[[O-(N-acetyl-\beta-neuraminosyl)-(2\rightarrow 3)-O-2,4,6-tris-O-(phenylmethyl)-\beta-D-galactopyranosyl-(1\rightarrow 4)-O-[6-deoxy-2,3,4-tris-O-(phenylmethyl)-\alpha-L-galactopyranosyl-(1\rightarrow 3)]-2-[(2-carboxybenzoyl)amino]-2-deoxy-6-O-(phenylmethyl)-<math>\beta$ -D-glucopyranosyl]oxy]- (9CI)

MF C92 H106 N2 O27

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN D-manno-2-Octulosonic acid, O- β -D-galactopyranosyl-(1+4)-O-2-(acetylamino)-2-deoxy- α -D-glucopyranosyl-(1+2)-O- β -D-glucopyranosyl-(1+4)-O-[O- α -D-galactopyranosyl-(1+4)-O- β -D-galactopyranosyl-(1+4)-O- α -D-glucopyranosyl-(1+2)- β -D-glucopyranosyl-(1+6)]-O-[β -D-glucopyranosyl-(1+3)]-O- α -D-glucopyranosyl-(1+5)-3-

PAGE 1-B

__ OH

Сн2− он

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,6-Octadienoic acid, 8-(β -D-glucopyranosyloxy)-3,7-dimethyl-, (E,E)- (9CI) MF C16 H26 O8

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Relative stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN Valeric acid, 5-(glucopyranosyloxy)- (8CI) MF C11 H20 08

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.04	47.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:18:48 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

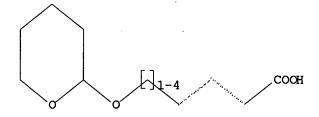
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 13:21:12 ON 30 NOV 2006 FILE 'REGISTRY' ENTERED AT 13:21:12 ON 30 NOV 2006 COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.04	47.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -2.25

Uploading c:\documents and settings\pzucker\my documents\examination auxillary files\10025947\10025947 refined1 st stab 8.6.06

L10 STRUCTURE UPLOADED

=> d 110 L10 HAS NO ANSWERS



STR

Structure attributes must be viewed using STN Express query preparation.

=> search 110 sss sam

SAMPLE SEARCH INITIATED 13:22:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 869 TO ITERATE

100.0% PROCESSED 869 ITERATIONS

0 ANSWERS

0 ANSWERS

-2.25

0.00

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

15612 TO 19148

PROJECTED ANSWERS:

0 TO

L11

0 SEA SSS SAM L10

=> search 110 sss full

FULL SEARCH INITIATED 13:22:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 16583 TO ITERATE

100.0% PROCESSED 16583 ITERATIONS

SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=> logoff hold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 174.42 215.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 13:22:24 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 13:31:50 ON 30 NOV 2006 FILE 'REGISTRY' ENTERED AT 13:31:50 ON 30 NOV 2006

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL SESSION
FULL ESTIMATED COST	SINCE FILE ENTRY 174.42	215.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.25
=> d hsi L12 HAS NO ANSWERS 'HSI ' IS NOT A VALID STRUCTURE FORMAT KEYWO'S Structure Formats SIA Structure Image, Attributes, and made data. (Default) SIM Structure IMage. SAT Structure ATtributes and map table SCT Structure Connection Table and map data. SDA All Structure DAta (image, attribute map table if it contains data). NOS NO Structure data. ENTER STRUCTURE FORMAT (SIM), NOS:d his 'D HIS' IS NOT A VALID STRUCTURE FORMAT KEYWO Structure Formats SIA Structure Image, Attributes, and made data. (Default) SIM Structure IMage. SAT Structure ATtributes and map table SCT Structure Connection Table and map data. SDA All Structure DAta (image, attribute map table if it contains data). NOS NO Structure data. ENTER STRUCTURE FORMAT (SIM), NOS:end	ap table if it con if it contains da table if it conta tes, connection ta ORD ap table if it con if it contains da table if it conta	ta. ins ble and tains tains
=> d his		
(FILE 'HOME' ENTERED AT 11:12:19 ON 30 I	NOV 2006)	
FILE 'REGISTRY' ENTERED AT 11:12:27 ON 3 L1 STRUCTURE UPLOADED L2 23 SEARCH L1 SSS SAM L3 STRUCTURE UPLOADED L4 9 SEARCH L3 SSS SAM E HEXANOIC ACID, 6-[(1-METHY) E HEXANOIC ACID, 6-((1-METHY) E 4-PHENYL-2-BUTYNOIC ACID/CI	L-2-PHENYL-1H-BENZ L-2-PHENYL-1H-BENZ	IMIDAZOL-6-YL)OXY IMIDAZOL-6-YL)OXY
L5 1 E3		
FILE 'CAPLUS' ENTERED AT 12:51:00 ON 30 L6 8 LO5 L7 3 L5	NOV 2006	
FILE 'REGISTRY' ENTERED AT 13:09:25 ON 3 E 5-TETRAHYDROPYRANYLOXY-2-PI L8 STRUCTURE UPLOADED L9 34 SEARCH L8 SSS SAM L10 STRUCTURE UPLOADED L11 0 SEARCH L10 SSS SAM L12 0 SEARCH L10 SSS FULL		·

=>

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L13 STRUCTURE UPLOADED

=> d 113 L13 HAS NO ANSWERS L13 STR

Structure attributes must be viewed using STN Express guery preparation.

=> search 113 sss sam
SAMPLE SEARCH INITIATED 13:32:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 66711 TO ITERATE

3.0% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

T EXCEEDED)

8 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1318840 TO 1349600 PROJECTED ANSWERS: 4356 TO 6316

L14 8 SEA SSS SAM L13

=> d scan

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN lH-Benzimidazole-1-pentanoic acid, 2-[4-[(4-carboxypentyl)oxy]phenyl]- α , α -dimethyl- (9CI)

MF C26 H32 N2 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C23 H20 C1 N O4 . Na

Na

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 3-[[(2S)-3-methyl-2-[[(1-naphthalenyloxy)acetyl]amino]-1-oxobutyl]amino]-4-oxo-5-(pentafluorophenoxy)-, (3S)- (9CI)

MF C28 H25 F5 N2 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 5-[3-[3-[(2R)-2-amino-2-phenylethyl]-1-[(2,6-difluorophenyl)methyl]-1,2,3,4-tetrahydro-6-methyl-2,4-dioxo-5-pyrimidinyl]-2-fluorophenoxy]- (9CI)

MF C31 H30 F3 N3 O5

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Octanoic acid, 8-[4-[[[1,2-dihydro-4-hydroxy-6-(2-naphthalenyl)-2-oxo-3-quinolinyl]carbonyl]amino]phenoxy]- (9CI)
MF C34 H32 N2 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 5-[(2'-hydroxy-5,5'-di-2-propenyl[1,1'-biphenyl]-2-yl)oxy](9CI)

MF C23 H26 O4

$$H_2C = CH - CH_2$$
 OH $H_2C = CH - CH_2$ O- $(CH_2)_4 - CO_2H$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 5-[2-(3-cyanopropyl)-6-(1,1-dimethylethyl)-4-[[3-ethoxy-5,7-dihydro-7-imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-

yl]acetyl]phenoxy]- (9CI) MF C32 H41 N5 O6 CI COM

MeNH-C NH
$$CH_2$$
-C CH_2) 3 $O-(CH_2)$ 4 $-CO_2H$ $Bu-t$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 5-[[3-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-1,2dihydro-7-methoxy-2-oxo-8-quinolinyl]oxy]- (9CI)

MF C24 H24 N2 O8

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 175.30 215.90 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -2.25

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:33:19 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

```
PASSWORD:
```

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 13:37:34 ON 30 NOV 2006
FILE 'REGISTRY' ENTERED AT 13:37:34 ON 30 NOV 2006
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COLINIGHT (C	2000 American Chen	itcar society (Ac	3)	
COST IN U.S.	DOLLARS		SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMAT	D COST		175.74	216.34
DISCOUNT AMO	NTS (FOR QUALIFYING	ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBE	R PRICE		0.00	-2.25
=> e 2-Pente E1	7,8,8A-OCTAHY	CID, 3-METHYL-5-	((4R, 4AR, 5S, 6R (HYDROXYMETHYL	8,8AS)-3,4,4A,5,6, 1)-2,5,8A-TRIMETHY
E2	2-PENTENOIC A 7,8,8A-OCTAHY	ACID, 3-METHYL-5- "DRO-5-(HYDROXYME"	((4R,4AR,5S,6R THYL)-2,5,8A-T	,8AS)-3,4,4A,5,6, RIMETHYL-4,6-BIS(
E3	(1-OXOPENTYL) 1> 2-PENTENOIC A -, (Z)-/CN	OXY)-1-NAPHTHALE CID, 3-METHYL-5-		
E4			((TETRAHYDRO-2	H-PYRAN-2-YL)OXY)
E5		CID, 3-METHYL-5-	((TETRAHYDRO-2	H-PYRAN-2-YL)OXY)
E6		CID, 3-METHYL-5-	((TETRAHYDRO-2	H-PYRAN-2-YL)OXY)
E7	1 2-PENTENOIC A ,5,5-TETRAMET			6,7-OCTAHYDRO-1,2 E),2B,
E8		'HYL-7-OXO-1-NAPH'		6,7-OCTAHYDRO-1,2 R-(1A(E),2.
E9	1 2-PENTENOIC A	CID, 3-METHYL-5- HYL-7-OXO-1-NAPH		6,7-OCTAHYDRO-1,2 THYL ESTER, (1R-(
E10	1 2-PENTENOIC A	CID, 3-METHYL-5- 5-TETRAMETHYL-1-1		6,7-OCTAHYDRO-7-H , METHYL ESTER, (
E11	1 2-PENTENOIC A			8,8A-OCTAHYDRO-1,
E12	1 2-PENTENOIC A	CID, 3-METHYL-5- L-5-METHYLENE-1-	(1,2,3,4,4A,5,	8,8A-OCTAHYDRO-1,
=> e3 L15	1 "2-PENTENOIC ACID (Z)-"/CN), 3-METHYL-5-((T	ETRAHYDRO-2H-P	YRAN-2-YL)OXY)-,
=> d 115				
RN 68420-7 ED Entered CN 2-Pente	OF 1 REGISTRY CO -3 REGISTRY STN: 16 Nov 1984 oic acid, 3-methyl- CA INDEX NAME)	-		xy]-, (Z)-
MF C11 H18 LC STN Fil	04		property data)	

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 182.84 223.44 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -2.25

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=> 115

L16 1 L15

=> d 116 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI Verrucarins and roridins. 35. Partial synthesis of tetrahydroverrucarin J

AN 1979:39055 CAPLUS

DN 90:39055

TI Verrucarins and roridins. 35. Partial synthesis of tetrahydroverrucarin J

AU Breitenstein, Werner; Tamm, Christoph
CS Inst. Org. Chem., Univ. Basel, Basel, Switz.
SO Helvetica Chimica Acta (1978), 61(6), 1975-83
CODEN: HCACAV; ISSN: 0018-019X
DT Journal

DT Journal
LA German

GI

Me H O H

II

AB Tetrahydroverrucarin (I) was prepared treating verrucarol monoacetate (II, R = Ac, R1 = H) with QOH [Q = 3-methyl-5-(tetrahydro-2H-pyran-2-yloxy)-2-pentanoyl], hydrolyzing II (R = Ac, R1 = Q), condensing II (R = H, R1 = Q) with HOQ1 [Q1 = p-BrC6H4CO2CO(CH2)4CO], hydrolyzing II (R = Q1,R1 = Q), and cyclizing II (R = R1 = H) in O-free xylene containing di-2-pyridyl disulfide and Ph3P.

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 4.12 227.56 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.75-3.00

FILE 'REGISTRY' ENTERED AT 13:40:04 ON 30 NOV 2006
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Ι

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8 DICTIONARY FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> e5

L17

1 "2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-"/CN

=> d 117

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 35066-34-3 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2-Pentenoic acid, 3-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Methyl trans-5-(tetrahydro-2-pyranyloxy)-3-methyl-2-pentenoate

FS STEREOSEARCH

MF C12 H20 O4

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 7.10 234.66

FULL ESTIMATED COST

CA SUBSCRIBER PRICE

SINCE FILE TOTAL ENTRY SESSION

-3.00

0.00

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=> d 117 1-3 ti fbib abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> 117

L18 3 L17

=> d 118 1-3 ti fbib abs

- L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI PtCl2-Catalyzed Transannular Cycloisomerization of 1,5-Enynes: A New Efficient Regio- and Stereocontrolled Access to Tricyclic Derivatives
- AN 2004:769838 CAPLUS
- DN 141:411094
- TI PtCl2-Catalyzed Transannular Cycloisomerization of 1,5-Enynes: A New Efficient Regio- and Stereocontrolled Access to Tricyclic Derivatives
- AU Blaszykowski, Christophe; Harrak, Youssef; Goncalves, Maria-Helena; Cloarec, Jean-Manuel; Dhimane, Anne-Lise; Fensterbank, Louis; Malacria, Max
- CS Laboratoire de Chimie Organique, Universite Pierre et Marie Curie, Paris, 75252, Fr.
- SO Organic Letters (2004), 6(21), 3771-3774 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 141:411094
- AB Transannular PtCl2-catalyzed cycloisomerizations open a new route to cyclopropanoic tricyclic systems. Ketones A or C were efficiently prepared from the same cycloundec-5-en-1-yne precursor B, depending on the substituent at the propargylic position (either benzoate or methoxy).
- RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Stereoselective synthesis of the macrocycle segment of verrucarin J
- AN 1982:103939 CAPLUS
- DN 96:103939
- TI Stereoselective synthesis of the macrocycle segment of verrucarin J
- AU White, James D.; Carter, J. Paul; Kezar, Hollis S., III
- CS Dep. Chem., Oregon State Univ., Corvallis, OR, 97331, USA
- SO Journal of Organic Chemistry (1982), 47(6), 929-32 CODEN: JOCEAH; ISSN: 0022-3263
- DT Journal
- LA English
- AB The ester acid, MeO2CCH:CMeCH2CH2O2C(CH:CH)2CO2H (2Z,7E,9Z-I), corresponding to the chain of verrucarin J, has been synthesized from HOCH2CH2COMe, whose tetrahydropyranyl ether was converted via a Wittig reaction to MeO2CCH:CMeCH2CH2OH. A Horner-Emmons condensation of MeO2CCH:CMeCH2CH2O2CCH2P(O)(OMe)2 derived from MeO2CCH:CMeCH2CH2Br and malonaldehydic acid gave 80% 2E,7E,9Z-I. A similar sequence from HOCH2CH2COMe via anhydromevalonolactone, gave the (Z)-phosphonate, which underwent a Horner-Emmons reaction to yield 2Z,7E,9Z-I. Comparison of 1H NMR spectra of I with data reported for verrucarin J confirms the revised 2E geometry assigned to the natural product.

- L18 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Metabolic products of microorganisms. 101. Synthesis of trans-5-hydroxy-3-methyl-2-pentenoic acid (trans-Δ2-anhydromevalonic acid)
- AN 1972:71960 CAPLUS
- DN 76:71960
- TI Metabolic products of microorganisms. 101. Synthesis of trans-5-hydroxy-3-methyl-2-pentenoic acid (trans-Δ2-anhydromevalonic acid)
- AU Keller-Schierlein, W.; Widmer, J.; Maurer, B.
- CS Org.-Chem. Lab., Eidg. Tech. Hochsch., Zurich, Switz.
- SO Helvetica Chimica Acta (1972), 55(1), 198-205 CODEN: HCACAV; ISSN: 0018-019X
- DT Journal
- LA German
- AB trans-Δ2-Anhydromevalonic acid (I) was prepared by treating 4-(tetrahydro-2-pyranyloxy)-2-butanone with Ph3P:CHCO2Me to give a mixture of mevalonic esters, which were separated after removal of the protective group and acetylation. Mild ammonolysis and alkaline saponification of trans-AcOCH2CH2CMe:CHCO2Me gave I. Condensation of AcOCH2CH2Ac with Ph3P:CHCO2Me gave Me 3-acetyl 4-methyl-3-cyclohexene-1-carboxylate, which on dehydration with S gave Me 3-acetyl-4-methylbenzoate.

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=> e 2-HexENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-/CN REG1stRY INITIATED Substance data EXPAND from CAS REGISTRY in progress...

E1	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
		INO)-, METHYL ESTER, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE
		R, $(E) - /CN$
E3	0>	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
		STER, (2E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
		STER, (E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
		ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
		ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		RIMETHYLSTANNYL) -, METHYL ESTER, (2) -/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
		YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
		YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN

=> e e1
 REG1stRY INITIATED
Substance data EXPAND from CAS REGISTRY in progress...

E1	1	2-HEXENOIC ACID, 6-((0-2,3,4-TRI-O-ACETYL-6-DEOXY-A-L-
		GALACTOPYRANOSYL-(1.FWDARW.3)-O-(O-2,3,4-TRI-O-ACETYL-6-DEOX Y-A-L-GALACTOPYRANOSYL-(1.FWDARW.2)-3,4,6-TRI-O-ACETYL
		-B-D-GALACTOPYR/CN
50	-	
E2	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
		INO)-, METHYL ESTER/CN
E3	1>	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
		INO)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE
		R_{\star} (E)-/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
		STER/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
		STER, (2E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
		STER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
	•	ESTER, (E)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
		ESTER, (Z)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
		YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
		, , , , , , , , , , , , , , , , , , , ,

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=> e e12		
E1	1 2-HEXENOI	C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		STANNYL)-, METHYL ESTER, (E)-/CN
E2		C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
		TANNYL)-, METHYL ESTER, (Z)-/CN
E3		C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
		L)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E4		C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E5		C ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
E6	YL ESTER/ 1 2-HEXENOT	
E0	/CN	CC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
E7	• • • • • • • • • • • • • • • • • • • •	C ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
L /	. METHYL	· · · · · · · · · · · · · · · · · · ·
E8		C ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES
20	TER/CN	o noisy o (1/1 simmill) i in similing, resimile is
E9	·	C ACID, 6-(1,2-DIHYDRO-4-HYDROXY-2-OXO-1-PHENYL-3-O
)-4,6-DIOXO-, ETHYL ESTER/CN
E10	1 2-HEXENOI	C ACID, 6-(1,2-DIHYDROXYCYCLOPENTYL)-3-(1-PYRROLIDI
	NYL)-, ME	THYL ESTER/CN
E11	1 2-HEXENOI	C ACID, 6-(1,3,3A,4,5,7A-HEXAHYDRO-6-METHYL-2H-INDE
•		NE)-3-METHYL-, METHYL ESTER, (2(Z),3A,7A.ALPH
	A.)-/CN	
E12		C ACID, 6-(1,3,3A,4,7,7A-HEXAHYDRO-1,3-DIOXO-4-ISOB
	ENZOFURAN	YL)-, METHYL ESTER/CN
=> e e1		
=> e e1 E1	1 2-HEXENOT	CONTRACTOR CONTRACTOR OF THE PROPERTY OF THE P
£Τ	ESTER, (E	C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
E2	•	C ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
56	ESTER, (2	
	DOTER, (Z	, , , ch

```
E3
             1 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
E4
                   RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E5
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
                   YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
E6
                   YLSTANNYL) -2-(TRIMETHYLGERMYL) -, METHYL ESTER, (Z)-/CN
E7
             1
                   2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
                   YL ESTER/CN
E8
             1
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
                   /CN
E9
             1
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
                   , METHYL ESTER/CN
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES
E10
             1
E11
             1
                   2-HEXENOIC ACID, 6-(1,2-DIHYDRO-4-HYDROXY-2-OXO-1-PHENYL-3-Q
                   UINOLINYL)-4,6-DIOXO-, ETHYL ESTER/CN
E12
             1
                   2-HEXENOIC ACID, 6-(1,2-DIHYDROXYCYCLOPENTYL)-3-(1-PYRROLIDI
                   NYL) -, METHYL ESTER/CN
=> e e1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E1
             1
                   STER, (2E) - /CN
E2
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
                   STER, (E) - /CN
E3
             1 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (E)-/CN
E4
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (Z) - / CN
E5
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
             1
E6
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E7
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
                   YLSTANNYL) -3-(TRIMETHYLGERMYL) -, METHYL ESTER, (E) -/CN
             1
E8
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
                   YLSTANNYL) -2-(TRIMETHYLGERMYL) -, METHYL ESTER, (Z)-/CN
E9
             1
                   2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
                   YL ESTER/CN
E10
             1
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
E11
             1
                   , METHYL ESTER/CN
E12
             1
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES
                   TER/CN
=> e e1
E1
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE
                   R, (E)-/CN
E2
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
                   STER/CN
             1 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E.3
                   STER, (2E) - /CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E4
                   STER, (E) - / CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (E) - /CN
E6
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (Z)-/CN
E7
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
             1
E8
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
```

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RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E9
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
                   YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E10
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
                   YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E11
             1
                   2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
                   YL ESTER/CN
E12
             1
                   2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
                   /CN
=> e e1
E1
             1
                   2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
                   INO) -, METHYL ESTER/CN
E2
             1
                   2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
                   INO)-, METHYL ESTER, (E)-/CN
E3
             1 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE
                   R, (E) -/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
             1
F.4
                   STER/CN
E5
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
                   STER, (2E)-/CN
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E6
                   STER, (E) - / CN
E7
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (E) - / CN
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
E8
                   ESTER, (Z)-/CN
E9
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
E10
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E11
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
                   YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
                   YLSTANNYL) -2-(TRIMETHYLGERMYL) -, METHYL ESTER, (Z) -/CN
=> e 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
E1
             1
                   2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AM
                   INO)-, METHYL ESTER, (E)-/CN
E2
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE
E3
             0 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E4
                   STER/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
E5
                   STER, (2E) - /CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
             1
E6
                   STER, (E) - /CN
E7
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
                   ESTER, (E) - / CN
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
E8
                   ESTER, (Z) - /CN
E9
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2.3-BIS(T
                   RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
E10
                   RIMETHYLSTANNYL) -, METHYL ESTER, (Z) -/CN
E11
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
                   YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12
             1
                   2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
                   YLSTANNYL) -2-(TRIMETHYLGERMYL) -, METHYL ESTER, (Z) -/CN
```

=> e 2-HEPtENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
E1 1 2-HEPTENOIC ACID, 7-((METHYLSULFONYL)OXY)-, METHYL ESTER/CN

E2	1	2-HEPTENOIC ACID, 7-((METHYLTHIO)THIOXOMETHOXY)-, ETHYL ESTE R, (E)-/CN
E3	0>	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
E4	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, 4-(1,3-DIOXOLAN-2-YL)BUTYL ESTER, (E)-/CN
E5	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E6	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E7	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E8	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-(±)-/CN
E9	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E10	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM ETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCL
		OHEXYL ESTER, (1R-(1A(Z),2B,5A))-/CN
E12	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM ETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ES TER, (1R-(1A(Z),2B,5A))-/CN

=> a cost		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	2.28	40.31
NETWORK CHARGES	0.36	6.30
SEARCH CHARGES	0.00	182.73
DISPLAY CHARGES	0.00	24.88
FULL ESTIMATED COST	2.64	254.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
the contraction of the golden and the contraction of the contraction o	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-5.25
ar bobbonizban rintol	0.00	3.23

IN FILE 'REGISTRY' AT 13:53:33 ON 30 NOV 2006

=> e e5		·
E1	1	The state of the s
		R, (E)-/CN
E2	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, 4-(1,3
		-DIOXOLAN-2-YL) BUTYL ESTER, (E)-/CN
E3	1>	2-HEPTENOIC ACID; 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL
		ESTER/CN
E4	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL
•		ESTER, (2E)-/CN
E5	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL
	_	ESTER, (E)-/CN
E6	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL
20	-	ESTER, $(E)-(\pm)-/CN$
E7	1	
E/	_	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
70	1	ESTER, (E)-/CN
E8	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
	_	ESTER, (Z)-/CN
E9	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM
		ETHYLSILYL) METHYL) -, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL) CYCL
		OHEXYL ESTER, (1R-(1A(Z),2B,5A))-/CN
E10	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM
		ETHYLSILYL) METHYL) 5-METHYL-2-(1-METHYLETHYL) CYCLOHEXYL ES

TER, (1R-(1A(Z), 2B, 5A))-/CN2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM E11 1 ETHYLSILYL) METHYL) -, ETHYL ESTER, (E) -/CN E12 2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM ETHYLSILYL) METHYL) -, ETHYL ESTER, (Z) -/CN => e5L19 1 "2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-"/CN => d 119

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

136277-38-8 REGISTRY

Entered STN: 20 Sep 1991 ED

2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester, (2E)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester, $(E) - (\pm) -$

OTHER NAMES:

2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester, CN

FS STEREOSEARCH

MF C14 H24 O4

SR

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplue 'CAPLUE' IS NOT A VALID FILE NAME SESSION CONTINUES IN FILE 'REGISTRY' Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue

accessing the remaining file names entered.

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 10.62 262.20 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -5.25 FILE 'CAPLUS' ENTERED AT 13:55:23 ON 30 NOV 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23 FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> 119

L20 2 L19

=> d 110 1-2 ti fbib abs

L10 HAS NO ANSWERS

'TI FBIB ABS ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ---- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ---- Structure IMage.

SAT ---- Structure ATtributes and map table if it contains data.

SCT ---- Structure Connection Table and map table if it contains data.

SDA ---- All Structure DAta (image, attributes, connection table and map table if it contains data).

NOS ---- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d 120 1-2 ti fbib abs

L20 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

TI A novel synthesis of the north west portion of Lasonolide A - an anticancer macrolide using Claisen rearrangement

AN 2005:184319 CAPLUS

DN 143:153204

TI A novel synthesis of the north west portion of Lasonolide A - an anticancer macrolide using Claisen rearrangement

AU Kar, Paramita; Rao, B. V.; Nagaiah, K.; Gurjar, M. K.

CS Organic Chemistry Division-III, Indian Institute of Chemical Technology, Hyderabad, 500 007, India

SO Journal of the Indian Chemical Society (2005), 82(1), 52-54 CODEN: JICSAH; ISSN: 0019-4522

PB Indian Chemical Society

DT Journal

LA English

OS CASREACT 143:153204

GT.

- AB A simplified analog of lasonolide A (C23-C35 side chain), I, was synthesized using Fujisawa's stereoselective variant of the Ireland Claisen ester rearrangement.
- RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L20 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Studies on the total synthesis of Pseudolaric acid A stereocontrolled synthesis of the seven-membered lactone
- AN 1999:446511 CAPLUS
- DN 131:272024
- TI Studies on the total synthesis of Pseudolaric acid A stereocontrolled synthesis of the seven-membered lactone
- AU Hu, You Hong; Ou, Li Gong; Wang, Xi Lu; Bai, Dong Lu
- CS Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, 200031, Peop. Rep. China
- SO Chinese Chemical Letters (1999), 10(4), 281-284 CODEN: CCLEE7; ISSN: 1001-8417
- PB Chinese Chemical Society
- DT Journal
- LA English
- OS CASREACT 131:272024
- GI

AB Pseudolaric acid A intermediate lactone I was obtained stereo- and regioselectively by a reaction sequence of 9 steps in 21% overall yield.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.78	269.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.50	-6.75

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http://www.cas.org/ONLINE/UG/regprops.html

=> e 2-HEXEN	NOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E1	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
	STER, (2E)-/CN
E2	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
	STER, (E)-/CN
_ E3	1> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
=4	ESTER, (E)-/CN
E4	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
77.E	ESTER, (Z)-/CN
E5	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
E6	RIMETHYLSTANNYL) -, METHYL ESTER, (E) -/CN 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2.3-BIS(T
EO	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E7	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
	YLSTANNYL) -3- (TRIMETHYLGERMYL) -, METHYL ESTER, (E)-/CN
E8	1 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
	YLSTANNYL) -2- (TRIMETHYLGERMYL) -, METHYL ESTER, (Z) -/CN
E9	1 2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
	YL ESTER/CN
E10	1 2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
	/CN
E11	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
	, METHYL ESTER/CN
E12	1 2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES
	TER/CN
=> e3	
L21	1 "2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
	ESTER, (E)-"/CN

=> d 121

```
L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
```

RN 127089-43-4 REGISTRY

ED Entered STN: 11 May 1990

CN 2-Hexenoic acid, 6-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H20 O4

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER (*File contains numerically searchable property data)

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 6 REFERENCES IN FILE CA (1907 TO DATE)
- 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 7.10 277.08 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -6.75

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=> 121

L22

6 L21

=> d 122 1-6 ti fbib abs

L22 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
TI Stereocontrolled Synthesis of Cyclic Ethers by Intramolecular

Hetero-Michael Addition. 5. Synthesis of All Diastereoisomers of 2,3,5,6-Tetrasubstituted Tetrahydropyrans

- AN 1997:416807 CAPLUS
- DN 127:95167
- TI Stereocontrolled Synthesis of Cyclic Ethers by Intramolecular Hetero-Michael Addition. 5. Synthesis of All Diastereoisomers of 2,3,5,6-Tetrasubstituted Tetrahydropyrans
- AU Betancort, Juan M.; Martin, Victor S.; Padron, Jose M.; Palazon, Jose M.; Ramirez, Miguel A.; Soler, Marcos A.
- CS Instituto Universitario de Bio-Organica Antonio Gonzalez, Universidad de La Laguna, Laguna, 38206 LA, Spain
- SO Journal of Organic Chemistry (1997), 62(14), 4570-4583 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 127:95167
- AB A systematic approach to the enantiomeric synthesis of all possible diastereoisomers of 2,6-dialkyl-3,5-dioxytetrahydropyrans is described. The key step is the intramol. cyclization of enantiomerically enriched (≥95% ee) 7-hydroxy-4-(benzoyloxy)-2,3-unsatd. esters. In fused systems, six of the eight diastereoisomers for one enantiomeric series were synthesized using this procedure. Using those with the suitable stereochem., the two left were synthesized by simple chemical transformations: in one case by the basic isomerization of the carbon with the (methoxycarbonyl) methyl substituent or by a Mitsunobu inversion of a secondary alc. available from the benzoyloxy group, in the remaining one by a consecutive sequence of oxidation and reduction reactions again over the free secondary alc. The stereochem. of the intramol. hetero-Michael addition leading to 2,3-disubstituted tetrahydropyrans is highly predictable when kinetic conditions (low temperature and sodium or potassium bases) are used and can be rationalized by invoking a model of a chair-like transition state in which the benzoyloxy group is located in the equatorial mode and the stereochem. course of the approach of the α,β -unsatd. ester is controlled by the geometry of the double bond. As a rule of thumb, the cyclization using E double bonds yielded cis-2,3-disubstituted tetrahydropyrans, while (Z)-unsatd. esters yielded the trans compds. This empirical rule is followed in highly substituted systems, leading to fused 2,3,5,6-tetrasubstituted tetrahydropyrans, with the same absolute configuration in the carbon where the nucleophilic oxygen is located and the one where the benzoyloxy group is located. Those systems having opposite configurations yield the same trans-2,3-disubstituted compound The isomerization under thermodn. conditions (room or higher temperature with

excess

of base) of the diastereoisomers with the (methoxycarbonyl)methyl substituent in the axial mode led quant. to those in which such a group was located equatorially. The scope and limitations of the method are described in both the synthesis of the unsatd. precursor and the stereochem. reached in the cyclization step.

- RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L22 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Intramolecular Diels-Alder reactions of internally-substituted trienylsulfones. Synthesis of bicyclo[4.3.0] and -[4.4.0] systems possessing a bridgehead sulfonyl group
- AN 1995:371268 CAPLUS
- DN 123:169270
- TI Intramolecular Diels-Alder reactions of internally-substituted trienylsulfones. Synthesis of bicyclo[4.3.0] and -[4.4.0] systems possessing a bridgehead sulfonyl group
- AU Clasby, Martin C.; Craig, Donald; Slawin, Alexandra M. Z.; White, Andrew J. P.; Williams, David J.

CS Dep. Chem., Imperial Coll. Sci., Technol. and Med., London, SW7 2AY, UK

SO Tetrahedron (1995), 51(5), 1509-32 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier

DT Journal

LA English

OS CASREACT 123:169270

AB A series of trienes possessing internally-activated vinylic sulfone dienophilic groups undergo intramol. Diels-Alder (IMDA) reaction with high or complete selectivity for the cis-fused products. Incorporation of silyloxy groups within the carbon tether linking the diene and dienophile results in increased IMDA reactivity. The stereochem. outcomes of these processes are rationalized in terms of the preference for an exo-oriented phenylsulfonyl group and a minimization of non-bonded interactions between the silyloxy and sulfone substituents.

L22 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

TI Stereoselective formation of trans-decalin and cis-decalin skeletons via hydroxy group directed cyclization induced by samarium(II) iodide

AN 1993:408384 CAPLUS

DN 119:8384

TI Stereoselective formation of trans-decalin and cis-decalin skeletons via hydroxy group directed cyclization induced by samarium(II) iodide

AU Kito, Makoto; Sakai, Toshinari; Yamada, Kaori; Matsuda, Fuyuhiko; Shirahama, Haruhisa

CS Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan

SO Symlett (1993), (2), 158-62 CODEN: SYNLES; ISSN: 0936-5214

DT Journal

LA English

OS CASREACT 119:8384

GΙ

AB By treating anti-hydroxy ketones, e.g., I, and syn-hydroxy ketones, e.g., II, with samarium(II) iodide, the ketone-olefin coupling cyclizations took place in a stereocontrolled manner to give the trans-decalin diol III and an epimeric mixts. of the cis-decalin diols, e.g., IV resp. The observed stereochemistries on the reductive coupling products are established by

chelation of the samarium(III) cation generated in the process, with the hydroxyl groups incorporated in the starting materials.

L22 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

TI Synthesis of ikarugamycin: model studies on a new strategy for the closure of ring C

AN 1990:611663 CAPLUS

DN 113:211663

TI Synthesis of ikarugamycin: model studies on a new strategy for the closure of ring C

AU Jones, Raymond C. F.; Jones, Richard F.

CS Chem. Dep., Nottingham Univ., Nottingham, NG7 2RD, UK

SO Tetrahedron Letters (1990), 31(23), 3367-8

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 113:211663

GI

AB A new conjugate addition-alkylation approach suitable for the closure of ring C of ikarugamycin is demonstrated by the concise elaboration of the trans-disubstituted cyclopentane I from (E)-MeO2CCH:CH(CH2)3I and LiCH2CO2CMe3. ABS: I has been converted into the cyclopentane analog of the natural product.

L22 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

TI Enantiomeric synthesis of endo-substituted tetrahydropyrans

AN 1990:497301 CAPLUS

DN 113:97301

TI Enantiomeric synthesis of endo-substituted tetrahydropyrans

AU Martin, Victor S.; Nunez, Maria T.; Ramirez, Miguel A.; Soler, Marcos A.

CS Cent. Prod. Nat. Org. "Antonio Gonzalez", Inst. Univ. Bio-Org., La Laguna, 38206, Spain

SO Tetrahedron Letters (1990), 31(5), 763-6

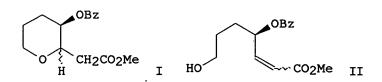
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 113:97301

GI



AB A general procedure for the enantioselective synthesis of 3-hydroxy-2-alkyltetrahydropyran benzoates I with absolute stereochem. control uses a new intramol. diastereoselective cyclization of chiral hydroxy- α , β -chiral unsatd. esters E- and Z-II. I are synthons

for the tetrahydropyran rings of the brevetoxins.

- L22 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
- TI A practical synthesis of (2E,6E,8E)-N-(2-methylpropyl)-2,6,8-hexadecatrien-10-ynamide
- AN 1990:216530 CAPLUS
- DN 112:216530
- TI A practical synthesis of (2E,6E,8E)-N-(2-methylpropyl)-2,6,8-hexadecatrien-10-ynamide
- AU Sharma, G. V. M.; Rajagopal, D.; Rao, E. Sreenivasa
- CS Div. Org. Chem. III, Indian Inst. Chem. Technol., Hyderabad, 500 007, India
- SO Synthetic Communications (1989), 19(18), 3181-9 CODEN: SYNCAV; ISSN: 0039-7911
- DT Journal
- LA English
- OS CASREACT 112:216530
- AB The title compound, derived from Achillea ageratifolia, was prepared from (E)-HOCH2CH:CHC.tplbond.CH via Wittig reaction of (E)-Me(CH2)4C.tplbond.CCH:CHCH2P+Ph3 Br- and (E)-MeO2CCH:CHCH2CH2CHO.

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	27.94	305.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-11.25

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:13:57 ON 30 NOV 2006

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Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	27.94	305.02
	·	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-11.25

=> save temp all tiredsrch/l

L# LIST L1-L22 HAS BEEN SAVED AS 'TIREDSRCH/L'

=> logoff hold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 28.86 305.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

-4.50 -11.25

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:27:12 ON 30 NOV 2006

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FULL ESTIMATED COST	28.86	305.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
43 Auna'ananan na 44	ENTRY	SESSION
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=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	28.86	305.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6 DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

1

5.0, AS/BI

E10

```
=> e 5-phenylpentynoic acid/cn
E1
             1
                   5-PHENYLPENTYLMETHYLAMINE/CN
E2
                   5-PHENYLPENTYLSULFONYL CHLORIDE/CN
E3
             0 --> 5-PHENYLPENTYNOIC ACID/CN
E4
                   5-PHENYLPHENAZIN-3-ONE/CN
E5
             1
                   5-PHENYLPHENAZINIUM PERCHLORATE/CN
E6
             1
                   5-PHENYLPHENAZINIUM, HYDROGEN SULFATE/CN
E7
                   5-PHENYLPHENOXYMETHYLPENICILLIN BENZYL ESTER/CN
             1
E8
             1
                   5-PHENYLPHENOXYMETHYLPENICILLIN K SALT/CN
F.9
             1
                   5-PHENYLPHENOXYMETHYLPENICILLIN SULFOXIDE BENZYL ESTER/CN
E10
             1
                   5-PHENYLPHTHALIMIDE/CN
E11
             1
                   5-PHENYLPIPERIDIN-3-OL/CN
E12
                   5-PHENYLPIPERIDINE-2, 4-DIONE/CN
=> logoff hold
COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                  TOTAL
                                                       ENTRY
                                                                SESSION
FULL ESTIMATED COST
                                                        0.88
                                                                 306.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                   TOTAL
                                                       ENTRY
                                                                 SESSION
CA SUBSCRIBER PRICE
                                                         0.00
                                                                  -11.25
 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:30:02 ON 30 NOV 2006
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LOGINID: SSSPTA1623PAZ
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SESSION RESUMED IN FILE 'REGISTRY' AT 14:33:59 ON 30 NOV 2006
FILE 'REGISTRY' ENTERED AT 14:33:59 ON 30 NOV 2006
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COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                  TOTAI.
                                                       ENTRY
                                                                SESSION
FULL ESTIMATED COST
                                                        0.88
                                                                 306.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                  SINCE FILE
                                                                  TOTAL
                                                       ENTRY
                                                                SESSION
CA SUBSCRIBER PRICE
                                                         0.00
                                                                  -11.25
=> e 5-phenylpentanoic acid
E1
             1
                   5-G/BI
E2
                   5-METHYL-2-PYRIDYL/BI
E3
             0 --> 5-PHENYLPENTANOIC ACID/BI
                   5-THREONINE/BI
E4
             1
E5
             1
                   5.,11/BI
E6
             1
                   5.,MO/BI
E7
           227
                   5.0/BI
                   5.0,AG/BI
E8
            3
             5
E9
                   5.0,AL/BI
```

```
E11
                   5.0,B/BI
E12
                   5.0,C/BI
=> e 5-phenylpentanoic acid/cn
E1
             1
                   5-PHENYLPENTANETHIOL/CN
E2
                   5-PHENYLPENTANOATE ION(1-)/CN
E3
             1 --> 5-PHENYLPENTANOIC ACID/CN
                   5-PHENYLPENTANOIC ACID (2-(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZO
E4
                   L-4-YL) ETHYL) AMIDE MONO (TRIFLUOROACETATE) / CN
E5
             1
                   5-PHENYLPENTANOIC ACID (4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-4
                   -YLMETHYL) AMIDE MONO (TRIFLUOROACETATE) / CN
E6
             1
                   5-PHENYLPENTANOIC ACID (4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-5
                   -YL) AMIDE HYDROCHLORIDE/CN
E7
             1
                   5-PHENYLPENTANOIC PERACID/CN
E8
             1
                   5-PHENYLPENTANOL/CN
E9
             1
                   5-PHENYLPENTANOYL CHLORIDE/CN
E10
             1
                   5-PHENYLPENTANOYLFERROCENE/CN
E11
             1
                   5-PHENYLPENTANOYLHYDROXAMIC ACID/CN
E12
             1 .
                   5-PHENYLPENTYL BROMIDE/CN
=> e3
L23
             1 "5-PHENYLPENTANOIC ACID"/CN
=> d 123
L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
     2270-20-4 REGISTRY
ED
     Entered STN: 16 Nov 1984
CN
     Benzenepentanoic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Valeric acid, \delta-phenyl- (4CI)
     Valeric acid, 5-phenyl- (6CI, 7CI, 8CI)
OTHER NAMES:
     \delta-Phenylvaleric acid
CN
     5-Phenylpentanoic acid
     5-Phenylvaleric acid
CN
CN
     NSC 65637
CN
     Phenylpentanoic acid
CN
     Phenylvaleric acid
MF
     C11 H14 O2
CI
     COM
LC
                  AGRICOLA, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD,
     STN Files:
       CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE,
       IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, RTECS*, SPECINFO, TOXCENTER.
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
                      EINECS**
         (**Enter CHEMLIST File for up-to-date regulatory information)
HO_2C-(CH_2)_4-Ph
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             461 REFERENCES IN FILE CA (1907 TO DATE)
              14 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             462 REFERENCES IN FILE CAPLUS (1907 TO DATE)
              22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
```

```
E1
                   5-PHENOXYPENT-3-YN-2-ONE/CN
            1
                  5-PHENOXYPENTANENITRILE/CN
E2
            1 --> 5-PHENOXYPENTANOIC ACID/CN
E3
            1
                5-PHENOXYPENTYL BROMIDE/CN
E4
E5
            1
                  5-PHENOXYPENTYL PHENYL KETONE/CN
E6
            1
                  5-PHENOXYPENTYLAMINE/CN
                 5-PHENOXYPENTYLMETHYLAMINE/CN
E7
            1
            1
                  5-PHENOXYPHENYLHYDRAZINE/CN
E8
               5-PHENOXYPIPERIDIN-3-OL/CN
E9
            1
           1
E10
                  5-PHENOXYSALICYLIC ACID/CN
           1
E11
                 5-PHENOXYTETRAZOLE/CN
           1
E12
                  5-PHENOXYTHIOPHENE-2-CARBOXALDEHYDE/CN
=> e3
            1 "5-PHENOXYPENTANOIC ACID"/CN
L24
=> d 124
L24 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
    7170-40-3 REGISTRY
ED
   Entered STN: 16 Nov 1984
CN Pentanoic acid, 5-phenoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Valeric acid, 5-phenoxy- (6CI, 7CI, 8CI)
OTHER NAMES:
     5-Phenoxypentanoic acid
     5-Phenoxyvaleric acid
CN
    NSC 192711
MF
    C11 H14 O3
CI
     COM
LC
                BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM,
     STN Files:
       SPECINFO, TOXCENTER, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
```

 $HO_2C-(CH_2)_4-OPh$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 44 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 44 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> 124

L25 44 L24

=> 124/prep

44 L24

4025189 PREP/RL

L26 11 L24/PREP

(L24 (L) PREP/RL)

=> d 126 5-11 ti fbib abs

L26 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of Grignard reagents from 3-halo ethers

AN 1983:575835 CAPLUS

DN 99:175835

TI Preparation of Grignard reagents from 3-halo ethers

AU Burns, Timothy P.; Rieke, Reuben D.

CS Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA

SO Journal of Organic Chemistry (1983), 48(22), 4141-3 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 99:175835

Treating PhO(CH2)3Br (I) with Mg turnings or highly reactive Mg powder in THF at room temperature followed by treatment with CO2 and hydrolysis gave PhOH and cyclopropane. Treating I with activated Mg (prepared according to R. D. Rieke, et al., 1981) in THF at -78° followed by treatment with CO2 and hydrolysis gave 71% PhO(CH2)3CO2H. PhO(CH2)nBr (n = 4-6) also formed stable Grignard reagents at low temps., but these reagents did not cyclize even in refluxing THF. Treating the reagents with CO2 followed by hydrolysis give 73-89% PhO(CH2)nCO2H.

L26 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Pseudo one-step cleavage of carbon-carbon bonds in the decomposition of ionized carboxylic acids. Radical-like reactions in mass spectrometry

AN 1983:125205 CAPLUS

DN 98:125205

TI Pseudo one-step cleavage of carbon-carbon bonds in the decomposition of ionized carboxylic acids. Radical-like reactions in mass spectrometry

AU Weiske, Thomas; Schwarz, Helmut

CS Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000/12, Fed. Rep. Ger.

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 98:125205

AB Metastable mol. ions of hexanoic acid (I) decompose unimol. to Et• and protonated methacrylic acid via intramol. H shift from C-3 or C-5 to the ionized carbonyl O; II is the essential intermediate. The gas-phase chemical of I cation radical, particularly H exchange between the CH2 groups C-2/C-3 and C-5/C-6, corresponds closely to the chemical of free alkyl radicals. The preparation of 13C- and D-labeled compds. is described.

L26 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Mass spectrometry in structural and stereochemical problems. CLXXIII. The electron impact induced fragmentations and rearrangements of trimethylsilyl esters of w-phenoxyalkanoic acids

AN 1969:523319 CAPLUS

DN 71:123319

TI Mass spectrometry in structural and stereochemical problems. CLXXIII. The electron impact induced fragmentations and rearrangements of trimethylsilyl esters of w-phenoxyalkanoic acids

AU Diekman, John; Thomson, James Bernard; Djerassi, Carl

CS Stanford Univ., Stanford, CA, USA

SO Journal of Organic Chemistry (1969), 34(10), 3147-61 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

In connection with the computer assisted interpretation of mass spectra, AΒ studies of the mass spectra of bifunctional compds. are needed in order to determine whether the electron impact-induced fragmentations are characteristic of each functional group or whether they reflect some interaction of the 2 In view of the wide applications of trimethylsilyl derivs. in combined vapor phase chromatog.-mass spectrometry, the mass spectra of a series of trimethylsilyl ω-phenoxyalkanoates were investigated. These mass spectra exhibit 4 prominent decomposition modes which depend upon the interaction of the Ph ether and silyl ester moieties. The mass spectra of some Ph, benzyloxy and alkoxy analogs as well as some Me ester analogs illustrate the necessity of the presence of a heteroatom in both of the functional groups at the ends of the polymethylene chain in order to observe the appropriate interactions. Since these seem to be rather independent of chain length, it is suggested that charge transfer involving the heteroatoms is responsible for maintaining the heteroatoms in close proximity, thus resulting in coiling of the polymethylene chain. The cleavages characteristic of each separate functionality in these compds. are also discussed.

L26 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Chloro carboxylic acids and some of their transformations

AN 1956:23982 CAPLUS

DN 50:23982

OREF 50:4849f-i,4850a-d

TI Chloro carboxylic acids and some of their transformations

AU Nesmeyanov, A. N.; Zakharkin, L. I.

CS Inst. Hetero-org. Compds., Acad. Sci., Moscow

SO Bulletin of the Academy of Sciences of the USSR, Division of Chemical Science (English Translation) (1955) 199-205 CODEN: BACCAT; ISSN: 0568-5230

DT Journal

LA English

cf. C.A. 49, 6120q. The tetrachloroalkanes used below were prepared from AΒ CC14 and C2H4 as described earlier. Cl(CH2)4CC13 was hydrolyzed to Cl(CH2)4CO2H; amide, m. 78-9°; anilide, m. 108-9°. Cl(CH2)6CCl3 was hydrolyzed to Cl(CH2)6CO2H; Et ester, bl1 122-3°, nD20 1.4392, d20 1.0110; anilide, m. 85-6°; amide, m. 82-3°. Cl(CH2)8CCl3 gave Cl(CH2)8CO2H, m. 29-30°; Et ester, b8 136-7°, nD20 1.4434, d20 0.9854; acyl chloride, b3 100-1°; amide, m. 76-7°; anilide, m. 95-6°; nitrile, b1.5 105-6°, nD20 1.4512, d20 0.9695. C1(CH2)10CC13, b3 141-2°, nD20 1.4822, d20 1.1558, heated with 92-3% H2SO4 1.5 hrs. at 100° gave 71.5% Cl(CH2)10CO2H, m. 41-2°, b1.5 149-51°; Et ester, b3 133-4°, nD20 1.4469, d20 0.9646; acyl chloride, b4.5 133-4°, amide, m. 89-90°; anilide, m. 69-70°; nitrile, b1.5 125-6°, nD20 1.4550, d20 0.9505. Cl (CH2) 12CCl3, b1.5 152-3°, nD20 1.4842, d20 1.1290, gave 42% Cl(CH2)12CO2H, m. 52-3°; Et ester, b1.5 147-9°, nD20 1.4535, d20 0.9604; acyl chloride, b1.5 146-7°; anilide, m. 70-1°. C1(CH2)14CCl3, b1 176-8°, nD20 1.4858, d20 1.1078, gave 24% Cl(CH2)14CO2H, m. 62-3°; Et ester, b1.5 168-70°, m. 31.5-2.5°; acyl chloride, b1.5 165-6°, m. 30-1°; anilide, m. 79-80°. Cl(CH2)4CO2Et heated with EtONa gave a little Et allylacetate and a good yield of EtO(CH2)4CO2Et, b10 87-8°, nD20 1.4225, d20 0.9386. Similarly Cl(CH2)6CO2Et gave EtO(CH2)6CO2Et, b1.5 77-8°, nD20 1.4292, d20 0.9290. NaCH(CO2Et)2 with Cl(CH2)4CO2Et in the presence of NaI in absolute EtOH gave in 6 hrs. 87% EtO2C(CH2)4CH(CO2Et)2, b2 147-9°, nD20 1.4389, d20 1.0568, hydrolyzed with 1:1 HCl to pimelic Similarly, Cl(CH2)6CO2Et gave 79% EtO2C(CH2)6CH(CO2Et)2, b1.5 169-70°, nD20 1.4419, d20 1.0316, hydrolyzed with HCl to azelaic acid. Refluxing Cl(CH2)8CO2H with PhOH in aqueous NaOH 3 hrs. gave 91% PhO(CH2)8CO2H, m. $69-70^{\circ}$; similarly was prepared PhO(CH2)6CO2H, m. 56-7°. Heating 20 g. δ -valerolactone with PhONa from 20 g. PhOH 4.5 hrs. at 200-10° gave on acidification 81% PhO(CH2)4CO2H, m. 65-6°, while NaSPh solution gave 65% PhS(CH2)4CO2H, m. 63-4°. Cl(CH2)6CO2H and NaCN in aqueous NaOH gave 63% NC(CH2)6CO2H, b1.5 145-7°, m. 39-40°, reduced with H over Raney Ni in 25% NH3 at $65-70^{\circ}$ and 90 atmospheric to H2N(CH2)7CO2H, m. $187-8^{\circ}$, in high yield. Heating C1(CH2)6CO2H with aqueous NaOH-Na2CO3 3 hrs. in an autoclave at 140-50° gave a good yield of HO(CH2)6CO2H, a sirup. Heating 18 g. Cl(CH2)6CO2H with 13.5 g. NaOH and 23 g. Me3N.HCl in 100 ml. H2O 3 hrs. in an autoclave at 130-40°, evaporating, and heating 1 hr. with 28 g. NaOH, finally to 185°, until Me3N evolution ceased, gave 10.1 g. CH2:CH(CH2)4CO2H, b14 118-20°, nD20 1.4400, d20 0.9500; p-toluidide, m. 60-1°; amide, m. 83-4°. Cl(CH2)4COCl (31 q.) in C6H6 treated with cooling with 28 g. AlCl3, the mixture allowed to stand 1 hr., refluxed 5 min., quenched in ice, and the organic layer washed with H2O gave 90% Cl(CH2)4Bz, m. 49-50°. Similarly was prepared 72% Cl (CH2) 6Bz, b1.5, 147-8°, m. 34-5°; 2,4dinitrophenylhydrazone, m. 110-11°. "C1(CH2)4CO2H in C6H6 with AlCl3 gave after 1 hr. on a steam bath 80% Ph(CH2)4CO2H," b1.5 132-3°, m. 59-60°; larger proportions of AlCl3 tend to produce also some α -benzosuberone, b7 124-5°, nD20 1.5618, d20 1.0780 (2,4-dinitrophenylhydrazone, m. 171-2°). C1(CH2)6CO2H similarly gave 76.5% PhCHMe(CH2)4CO2H, b3 165-6°, nD20 1.5089, d20 1.0206; amide, m. 55.5-6.5°. Cl(CH2)8CO2H gave PhCHMe(CH2)6CO2H, b1 155-7°, nD20 1.5043, d20 0.9957; oxidation gave AcPh. Similarly was prepared PhCHMe(CH2)8CO2H, b3 186-8°, nD20 1.5005, d20 0.9779.

L26 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
TI Chloro carboxylic acids and some of their transformations
AN 1956:23981 CAPLUS
DN 50:23981
OREF 50:4849f-i,4850a-d

Chloro carboxylic acids and some of their transformations TI

Nesmeyanov, A. N.; Zakharkin, L. I. AU

Inst. Hetero-org. Compds., Acad. Sci., Moscow CS

Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1955) 224-32 SO CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LΑ Unavailable

cf. C.A. 49, 6120g. The tetrachloroalkanes used below were prepared from AB CC14 and C2H4 as described earlier. C1(CH2)4CC13 was hydrolyzed to Cl(CH2)4CO2H; amide, m. 78-9°; anilide, m. 108-9°. Cl(CH2)6CCl3 was hydrolyzed to Cl(CH2)6CO2H; Et ester, b11 122-3°, nD20 1.4392, d20 1.0110; anilide, m. 85-6°; amide, m. 82-3°. Cl(CH2)8CCl3 gave Cl(CH2)8CO2H, m. 29-30°; Et ester, b8 136-7°, nD20 1.4434, d20 0.9854; acyl chloride, b3 100-1°; amide, m. 76-7°; anilide, m. 95-6°; nitrile, b1.5 105-6°, nD20 1.4512, d20 0.9695. C1(CH2)10CCl3, b3 141-2°, nD20 1.4822, d20 1.1558, heated with 92-3% H2SO4 1.5 h. at 100° gave 71.5% Cl(CH2)10CO2H, m. 41-2°, b1.5 149-51°; Et ester, b3 133-4°, nD20 1.4469, d20 0.9646; acyl chloride, b4.5 133-4°, amide, m. 89-90°; anilide, m. 69-70°; nitrile, b1.5 125-6°, nD20 1.4550, d20 0.9505. Cl(CH2)12CCl3, b1.5 152-3°, nD20 1.4842, d20 1.1290, gave 42% C1(CH2)12CO2H, m. 52-3°; Et ester, b1.5 147-9°, nD20 1.4535, d20 0.9604; acyl chloride, b1.5 146-7°; anilide, m. 70-1°. C1(CH2)14CCl3, b1 176-8°, nD20 1.4858, d20 1.1078, gave 24% Cl(CH2)14CO2H, m. 62-3°; Et ester, b1.5 168-70°, m. 31.5-2.5°; acyl chloride, b1.5 165-6°, m. 30-1°; anilide, m. 79-80°. Cl(CH2)4CO2Et heated with EtONa gave a little Et allylacetate and a good yield of EtO(CH2)4CO2Et, bl0 87-8°, nD20 1.4225, d20 0.9386. Similarly Cl(CH2)6CO2Et gave EtO(CH2)6CO2Et, b1.5 77-8°, nD20 1.4292, d20 0.9290. NaCH(CO2Et)2 with C1(CH2)4CO2Et in the presence of NaI in absolute EtOH gave in 6 h. 87% EtO2C(CH2)4CH(CO2Et)2, b2 147-9°, nD20 1.4389, d20 1.0568, hydrolyzed with 1:1 HCl to pimelic acid. Similarly, Cl(CH2)6CO2Et gave 79% EtO2C(CH2)6CH(CO2Et)2, b1.5 169-70°, nD20 1.4419, d20 1.0316, hydrolyzed with HCl to azelaic acid. Refluxing Cl(CH2)8CO2H with PhOH in aqueous NaOH 3 h. gave 91% PhO(CH2)8CO2H, m. 69-70°; similarly was prepared PhO(CH2)6CO2H, m. 56-7°. Heating 20 g. δ-valerolactone with PhONa from 20 g. PhOH 4.5 h. at 200-10° gave on acidification 81% PhO(CH2)4CO2H, m. 65-6°, while NaSPh solution gave 65% PhS(CH2)4CO2H, m. 63-4°. Cl(CH2)6CO2H and NaCN in aqueous NaOH gave 63% NC(CH2)6CO2H, b1.5 145-7°, m. 39-40°, reduced with H over Raney Ni in 25% NH3 at $65-70^{\circ}$ and 90 atmospheric to H2N(CH2)7CO2H, m. $187-8^{\circ}$, in high yield. Heating Cl (CH2) 6CO2H with aqueous NaOH-Na2CO3 3 h. in an autoclave at 140-50° gave a good yield of HO(CH2)6CO2H, a sirup. Heating 18 g. Cl(CH2)6CO2H with 13.5 g. NaOH and 23 g. Me3N.HCl in 100 mL. H2O 3 h. in an autoclave at 130-40°, evaporating, and heating 1 h. with 28 g. NaOH, finally to 185° , until Me3N evolution ceased, gave 10.1~g. CH2:CH(CH2)4CO2H2 b14 118-20°, nD20 1.4400, d20 0.9500; p-toluidide, m. 60-1°; amide, m. 83-4°. C1(CH2)4COC1 (31 g.) in C6H6 treated with cooling with 28 g. AlCl3, the mixture allowed to stand 1 h., refluxed 5 min., quenched in ice, and the organic layer washed with H2O gave 90% Cl(CH2)4Bz, m. 49-50°. Similarly was prepared 72% Cl(CH2)6Bz, b1.5, 147-8° m. 34-5°; 2,4-dinitrophenylhydrazone, m. 110-11°. "Cl(CH2)4CO2H in C6H6 with AlCl3 gave after 1 h. on a steam bath 80% Ph(CH2)4CO2H, b1.5 132-3°, m. 59-60°; larger proportions of AlCl3 tend to produce also some α -benzosuberone, b7 124-5°, nD20 1.5618, d20 1.0780 (2,4-dinitrophenylhydrazone, m. 171-2°). C1(CH2)6CO2H similarly gave 76.5% PhCHMe(CH2)4CO2H, b3 165-6°, nD20 1.5089, d20 1.0206; amide, m. 55.5-6.5°. Cl(CH2)8CO2H gave PhCHMe(CH2)6CO2H, b1 155-7°, nD20 1.5043, d20 0.9957; oxidation gave AcPh. Similarly was prepared PhCHMe(CH2)8CO2H, b3 186-8°, nD20 1.5005, d20 0.9779.

L26 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN Synthetical experiments relating to carpaine. III. Some derivatives of tetrahydrofuran and intermediates of the aliphatic series AN 1937:38106 CAPLUS DN 31:38106 OREF 31:5351i,5352a-g Synthetical experiments relating to carpaine. III. Some derivatives of tetrahydrofuran and intermediates of the aliphatic series Barger, G.; Robinson, Robert; Smith, Leonard H. Journal of the Chemical Society (1937) 718-25 SO CODEN: JCSOA9; ISSN: 0368-1769 DT Journal Unavailable LΑ CASREACT 31:38106 os AΒ Tetrahydrofurfuryl chloride is surprisingly inert toward KCN and AccHNaCO2Et and even the bromide (I) could not be condensed with the latter reagent in Et2O, EtOH, dioxane, PhMe or C6H6; with CHNa-(CO2Et)2 there results 70% of Et tetrahydrofurfurylmalonate (II), b1 123°; hydrolysis and decarboxylation give β -tetrahydrofurylpropionic acid, b0.2 119° nD15 1.4591; Et ester, b11, 105°, nD15 1.4425. Reduction gives 75% of 3-tetrahydrofurylpropan-1-ol, b11 111.5°, nD13 1.4597; the chloride bl1, 78° ; the bromide (III) bl6 100-1°. II and III with EtONa in EtOH, refluxed 30 h., give Et bis(tetrahydrofurfuryl)malonate, b0.5 165°, yielding on hydrolysis and decarboxylation β,β' -bis(tetrahydrofurfuryl)-isobutyric acid, b0.35 173°. Tetrahydrofurfuryl p-toluene-sulfonate, m. 38.7-9.1°. Refluxing 30 g. I, 20 g. KCN and 1 g. NaI in dilute EtOH for 35 h. gives 7 g. tetrahydro-furylacetonitrile, b13 92.4°, nD13 1.4476; hydrolysis of 10 g. gives 7.7 g. tetrahydrofurylacetic acid, b16 144-6°. II and 11-bromoundecanyl acetate in EtOH-EtONa, refluxed 5 h., followed by hydrolysis, yield 12,12-dicarboxy-13tetrahydrofuryltridecan-1-ol, m. $108-9^{\circ}$. Details are given of the preparation of Et 2-furoylacetate in 93% yield from Et furoate, AcOEt and Na; b1, 113-14°, nD16 1.5055. Et 6-hydroxyhexoate (IV) (10 g.) and SOC12 in C5H5N give 9.1 g. of the 6-Cl derivative, b14 106°, nD18 1.4398; the 6-Br derivative (V) (with PBr3 in C5H5N) b21 $126-7^{\circ}$; it is more satisfactorily prepared by using HBr and reesterifying (31 g. from 30 g. IV), although there is some question as to the homogeneity of the product, because isomerization may occur by way of an ethylene derivative It is suggested that such reactions should be effected in the presence of O2 and peroxide catalysts. Et 7-bromoheptoate (VI), b17 135°. Refluxing 31 g. V and 17.5 g. AcCH2CO2Et with EtONa for 9 h. gives 18 g. Et α -acetylsuberate, b0.28 154-8°; shaking with KOH at room temperature gives 8-ketononoic acid, m. 40-1°; 2,4dinitrophenylhydrazone, yellow, m. 88-9°; semicarbazone, m. 136°; Et ester (VII), b11 141-2° (semicarbazone, m. 108°); p-phenylphenacyl ester, m. 93.5-5°. VI (25 g.) and AcCH2CO2Et give 18 g. crude Et α-acetylazelate, yielding with KOH 91.5% of 9-ketodecoic acid, m. 47.5-8.5°; semicarbazone, with 2 mols. H2O, m. 127° (anhydrous; from aqueous MeOH, m. 115-16°); Et ester, bl1 154-6° (semicarbazone, m. 97-8°); p-phenylphenacyl ester, m. 68-70°. VII and AmMgBr give 8-hydroxy-8-methyltridecoic acid, isolated as the p-phenylphenacyl ester, m. 68-71°. AcCH2CO2Et and PhO(CH2)3Br with EtONa give 71% of Et γ-phenoxy-propylacetoacetate (VIII), b1, 164°, nD18; 1.5018; there also resulted Et bis(phenoxypropyl)acetoacetate, m. 61-2°. VIII (98.5 g.) and MeO2C(CH2)2COCl, refluxed 16 h. and hydrolyzed with KOH, give 22.5 g. of Me δ -phenoxybutyl ketone, pale lemon oil, bl 136-7°, nD13 1.5143 (2,4-dinitrophenylhydrazone, yellow, m. 97-8°); 8.5 g. of Et 5-phenoxyvalerate, b0.42 115-17° and 3 g. of the Et ester, $b0.42 135-40^{\circ}$, of 8-phenoxyoctoic acid, m.

68-70°. Hydrolysis of VIII gives 5-phenoxyvaleric acid, whose

anilide m. 84.5-5.5°.

L26 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Synthesis of heptane-1,5-dicarboxylic acid

AN 1928:26986 CAPLUS

DN 22:26986

OREF 22:3137a-b

TI Synthesis of heptane-1,5-dicarboxylic acid

AU Carter, Albert S.

CS Univ. Wisconsin

SO Journal of the American Chemical Society (1928), 50, 1967-70 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

OS CASREACT 22:26986

AB Di-Et γ-phenoxypropylmalonate, b26 228-35°, results in 76% yield from CH2(CO2Et)2, PhO(CH2)3Br and Na; the free acid m. 72-8° (90% yield); heating at 175° gives 90% of PhO(CH2)4CO2H, m. 55-6°; HI gives 60% of I(CH2)4CO2H, whose Et ester b20 108-18°; with EtCH(CO2Et)2 and Na this gives the tri-Et ester, b20 192-200°, of heptane-1,5,5-tricarboxylic acid, m. 86-8°, decomps. 140°, giving heptane-1,5-dicarboxylic acid, m. 41.5-3°, analyzed as the Ag salt.

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E4
                   5-PHENOXY-2-PHENYL-1,3,4-OXADIAZOLE/CN
E5
                   5-PHENOXY-2-THENYL ALCOHOL/CN
E6
             1
                   5-PHENOXY-2-THIOPHENEMETHANOL/CN
F.7
             1
                   5-PHENOXY-3, 4, 6-TRICHLOROPYRIDAZINE/CN
E8
             1
                   5-PHENOXY-3, 4-DIHYDRO-1H-QUINAZOLIN-2-ONE/CN
E9
            1
                   5-PHENOXY-3-((4,5,7-TRIFLUOROBENZOTHIAZOL-2-YL)METHYL)INDOLE
                   -N-ACETIC ACID/CN
E10
             1
                   5-PHENOXY-3-(A-HYDROXYETHYL) PYRIDINE/CN
E11
             1
                   5-PHENOXY-3-(2-(4-BENZYLPIPERAZIN-1-YL)ETHYL)INDOLE/CN
E12
                   5-PHENOXY-3-(2-(4-PYRIDINYL)-1,3-THIAZOL-4-YL)-2(1H)-PYRIDIN
                   ONE/CN
=> e 6-phenoxy-2-hexenoic acid/cn
                   6-PHENOXY-2-((4-PHENOXYPHENYL)AMINO)-4H-THIENO(2,3-D)(1,3)OX
                   AZIN-4-ONE/CN
E2
                   6-PHENOXY-2-BENZOFURANCARBOXYLIC ACID/CN
E3
             0 --> 6-PHENOXY-2-HEXENOIC ACID/CN
E4
                   6-PHENOXY-2-HYDROXYHEXANOIC ACID/CN
E5
            1
                   6-PHENOXY-2-OXOHEXANOIC ACID/CN
                   6-PHENOXY-2-PYRIDINECARBOTHIOAMIDE/CN
E6
            1
E7
            1
                   6-PHENOXY-2-PYRIDINECARBOXALDEHYDE/CN
E8
            1
                   6-PHENOXY-2-PYRIDINECARBOXYLIC ACID/CN
E9
            1
                   6-PHENOXY-2-PYRIDINEMETHANETHIOL/CN
            1
E10
                   6-PHENOXY-2-PYRIDINEMETHANOL/CN
            1
E11
                   6-PHENOXY-3-PYRIDINAMINE/CN
            1
E12
                   6-PHENOXY-3-PYRIDINAMINE HYDROCHLORIDE/CN
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COST IN U.S. DOLLARS
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FULL ESTIMATED COST
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                                                       ENTRY
                                                                SESSION
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        SEP 21
NEWS
     7
                CA/CAplus fields enhanced with simultaneous left and right
                truncation
NEWS 8 SEP 25 CA(SM)/Caplus(SM) display of CA Lexicon enhanced
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NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine. NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new classification scheme NEWS 12 OCT 19 LOGOFF HOLD duration extended to 120 minutes NEWS 13 OCT 19 E-mail format enhanced Option to turn off MARPAT highlighting enhancements available NEWS 14 OCT 23 NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in multiple databases NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality NEWS 19 NOV 10 CA/CAplus F-Term thesaurus enhanced NEWS 20 NOV 10 STN Express with Discover! free maintenance release Version 8.01c now available NEWS 21 NOV 13 CA/Caplus pre-1967 chemical substance index entries enhanced with preparation role NEWS 22 NOV 20 CAS Registry Number crossover limit increased to 300,000 in additional databases NEWS 23 NOV 20 CA/Caplus to MARPAT accession number crossover limit increased to 50,000 NEWS 24 NOV 20 CA/CAplus patent kind codes will be updated NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT

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SINCE FILE TOTAL
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0.21

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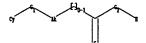
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=>

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chain nodes:
1 2 3 4 5 6 7 9

chain bonds :

1-2 2-3 3-4 4-5 5-6 5-9 6-7

exact/norm bonds :

1-2 2-3 3-4 5-6 5-9 6-7

exact bonds :

4-5

G1:CH2,O,S,N

G2:0,S

Hydrogen count :
4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS Generic attributes :

3:

Type of chain Saturation

: Linear : Unsaturated

Saturation

Element Count : Node 3: Limited C,C5-12

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

STR

$$Cy$$
 Ak $G2$ H

G1 CH2, O, S, N

G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 05:51:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1309181 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

26125935 TO 26241305

PROJECTED ANSWERS:

36617 TO 41933

3 ANSWERS

L2 3 SEA SSS SAM L1

=> dscan

0 DSCAN

L3

0 DSCAN

=> d scan 12

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Heptenoic acid, 7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxy-5-(3-methoxyphenyl)-1-penten-4-ynyl]cyclopentyl]-, (5Z)- (9CI)

MF C24 H30 O6

Absolute stereochemistry.

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Heptenoic acid, $7-[2-[4-(3-\text{chlorophenoxy})-3-\text{hydroxy}-4-\text{methyl}-1-\text{pentenyl}]-3-\text{hydroxy}-5-\text{oxocyclopentyl}]-, methyl ester, [1R-[1<math>\alpha$ (Z),2 β (1E,3R*),3 α]]- (9CI)

MF C25 H33 C1 O6

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Octenoic acid, 8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5-yl]-, [2 α ,4 α ,5 α (Z)]-, compd. with 1,2-ethanediamine (9CI)

MF C19 H23 F3 O5 . \times C2 H8 N2

CM 1

Relative stereochemistry. Double bond geometry as shown.

CM 2

 $H_2N-CH_2-CH_2-NH_2$

ALL ANSWERS HAVE BEEN SCANNED

=>

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chain nodes :
2 3 4 5 6 7 9
ring nodes :

1 16 17 18 19 20

chain bonds :

1-2 2-3 3-4 4-5 5-6 5-9 6-7

ring bonds :

1-16 1-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 3-4 5-6 5-9 6-7

exact bonds :

4-5

normalized bonds :

1-16 1-20 16-17 17-18 18-19 19-20

G1:CH2,O,S,N

G2:0,S

Hydrogen count :
4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 16:Atom

17:Atom 18:Atom 19:Atom 20:Atom

Generic attributes :

3:

Type of chain

: Linear

Saturation

: Unsaturated

Element Count : Node 3: Limited C,C5-12

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4

STR

G1 CH2, O, S, N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search 14 sss sam

SAMPLE SEARCH INITIATED 05:57:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 958287 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

INCOMPLETE BATCH

PROJECTED ITERATIONS: 19113707 TO 19217773 0

PROJECTED ANSWERS: 0 TO

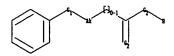
L5 0 SEA SSS SAM L4

=> d cost COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION CONNECT CHARGES 5.32 5.47 **NETWORK CHARGES** 0.84 0.90 SEARCH CHARGES 4.76 4.76 FULL ESTIMATED COST 10.92 11.13

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chain nodes : 2 3 4 5 6

ring nodes :

1 16 17 18 19 20

chain bonds :

1-2 2-3 3-4 4-5 5-6 5-9 6-7

ring bonds :

1-16 1-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 3-4 5-6 5-9 6-7

exact bonds :

4-5

normalized bonds :

1-16 1-20 16-17 17-18 18-19 19-20

G1:CH2,O,S,N

G2:0,S

Hydrogen count :
4:>= minimum 2
Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 16:Atom

17:Atom 18:Atom 19:Atom 20:Atom

Generic attributes :

3:

Type of chain : Linear Saturation : Unsaturated

Element Count : Node 3: Limited C,C5-12

L6 STRUCTURE UPLOADED

=> d 16 L6 HAS NO ANSWERS L6 STR

G1 CH2, O, S, N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search 16 sss sam

SAMPLE SEARCH INITIATED 05:59:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 958287 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

19113707 TO 19217773 PROJECTED ITERATIONS: PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> search 16 sss full FULL SEARCH INITIATED 06:00:48 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 19162978 TO ITERATE

| 0.7% | PROCESSED | 125825 | ITERATIONS | | | | 7 | ANSWERS |
|---------|---|---------|---------------------------|-----------|---|-------------|----|---------|
| 1.4% | PROCESSED | 260970 | ITERATIONS | (| 3 | INCOMPLETE) | 16 | ANSWERS |
| 2.0% | PROCESSED | 388633 | ITERATIONS | (| 3 | INCOMPLETE) | 28 | ANSWERS |
| 3.3% | PROCESSED | 624718 | ITERATIONS | (| 4 | INCOMPLETE) | 34 | ANSWERS |
| 3.7% | PROCESSED | 705315 | ITERATIONS | (| 4 | INCOMPLETE) | 36 | ANSWERS |
| 4.2% | PROCESSED | 797752 | ITERATIONS | (| 4 | INCOMPLETE) | 37 | ANSWERS |
| 4.78 | PROCESSED | 902887 | ITERATIONS | (| 6 | INCOMPLETE) | 91 | ANSWERS |
| 5.0% | PROCESSED | 962254 | ITERATIONS | (| 6 | INCOMPLETE) | 91 | ANSWERS |
| INCOMPI | PROCESSED
LETE SEARCH
TIME: 00.02 | (SYSTEM | ITERATIONS
LIMIT EXCES | (
DED) | 6 | INCOMPLETE) | 91 | ANSWERS |

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 19162978 TO 19162978

PROJECTED ANSWERS: 1618 TO 1868

L8 91 SEA SSS FUL L6

=> d scan

rs91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,4-Decadienoic acid, 6,6,7,7,8,8,9,9,10,10,10-undecafluoro-5-(4-

methoxyphenoxy)-, methyl ester, (2E,4E)- (9CI)

C18 H13 F11 O4 MF

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-(2-hydroxy-5methoxyphenyl) - (9CI)

MF C25 H23 F O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2006 ACS on STN L8 91 ANSWERS

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[(5methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]- (9CI)

MF C36 H32 F N O6

F

$$CO_2H$$
 $CH_2-CH_2-CH_2-CH_2-CH_2$
 CH_2-O
 CH_2-O

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2006 ACS on STN r_8 91 ANSWERS

5-Hexenoic acid, 2-(4-bromophenoxy)-6-phenyl-, ethyl ester (9CI) IN

MF C20 H21 Br O3

$$\begin{array}{c} \circ \\ \parallel \\ \mathsf{C-OEt} \\ - \\ \mathsf{O-CH-CH}_2-\mathsf{CH}_2-\mathsf{CH} \\ = \mathsf{CH-Ph} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

The image of the image of

MF C29 H40 O8 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE
- IN Poly[oxy[5-[[pentakis[[4-[2-[2-(2-ethoxyethoxy)ethoxy]ethoxy]phenyl]ethyny
 l]phenyl]ethynyl]-1,3-phenylene]oxy(1,14-dioxo-1,14-tetradecanediyl)]
 (9CI)
- MF (C108 H132 O24)n
- CI PMS

RELATED POLYMERS AVAILABLE WITH POLYLINK

PAGE 1-A

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Heptenoic acid, 6-oxo-7-phenyl-, phenylmethyl ester (9CI)

MF C20 H20 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-phenyl- (9CI)

MF C24 H21 F O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-fluorophenyl]-2-(2-methoxyphenoxy)- (9CI)

MF C28 H30 F N O5

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C33 H32 F3 N O6

$$\begin{array}{c} O \\ C \\ C \\ O \\ CH \\ CH_2 \\ CH_2 \\ O \\ \end{array} \begin{array}{c} O \\ CH_2 \\ O \\ \end{array} \begin{array}{c} O \\ O \\ Me \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C30 H40 O2 S

Double bond geometry as shown.

PAGE 1-A

Et Z

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN Cholest-5-en-3-ol (3β) -, 13-[2,3-difluoro-4-[(1E)-[4-(octyloxy)phenyl]azo]phenoxy]tridecanoate (9CI)

MF C60 H92 F2 N2 O4

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

Me
$$(CH_2)_{7}$$
 $(CH_2)_{12}$ $(CH_2)_{12}$

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)

MF C34 H34 F3 N O6

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-methylphenyl]-2-(2-methoxyphenoxy)- (9CI)

MF C29 H33 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-, ethyl ester (9CI)

MF C30 H31 F3 O6

MeO
$$CH = CH - CH_2 - CH_2 - CH - O$$
 CF_3

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 8-Dodecenoic acid, 12-[3-methoxy-4-(methoxymethoxy)phenyl]-10-oxo-, ethylester (9CI)

MF C23 H34 O6

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,4-Heptadienoic acid, 7-(4-methoxyphenoxy)-, ethyl ester, (2E,4E)- (9CI)

MF C16 H20 O4

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-[4-(trifluoromethyl)phenoxy]- (9CI)

MF C20 H19 F3 O5

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]1-oxo-1H-inden-5-yl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-, ethyl ester
(9CI)

MF C40 H36 F N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[4-(5-chloro-2-thienyl)phenoxy]-6-phenyl- (9CI)

MF C22 H19 C1 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Hexenoic acid, 6-(2-iodophenoxy)-, ethyl ester, (2E)- (9CI)

MF C14 H17 I O3

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

- L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE
- IN Poly[oxy[5-[[pentakis[(4-dodecylphenyl)ethynyl]phenyl]ethynyl]-1,3-phenylene]oxy(1,14-dioxo-1,14-tetradecanediyl)] (9CI)
- MF (C128 H172 O4)n
- CI PMS

RELATED POLYMERS AVAILABLE WITH POLYLINK

- L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN 2-Heptenoic acid, 6-hydroperoxy-6-methoxy-7-phenyl-, phenylmethyl ester (9CI)
- MF C21 H24 O5

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-(4-bromophenoxy)-6-phenyl- (9CI)

MF C18 H17 Br O3

$$CO_2H$$
 $O-CH-CH_2-CH_2-CH=CH-Ph$
Br

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4-

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)

MF C15 H17 F3 O3

$$\begin{array}{c|c} & \circ & \circ \\ \parallel & \circ & \circ \\ \text{Eto-C} & \circ & \circ \\ \parallel & \circ & \circ \\ \text{H}_2\text{C} = \text{CH-CH}_2 - \text{CH}_2 - \text{CH-O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2,4-Octadienoic acid, 8-[4-[2-[5-(acetylamino)-2,2-dimethyl-1,3-dioxan-5-

yl]ethyl]phenyl]- (9CI) MF C24 H33 N O5

Me O
$$CH_2-CH_2$$
 CH_2-CH_2 CH_2-CH_2 CH_2-CH_2 CH_2-CH_2 CH_2-CH_2 CH_2-CH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

$$V_{\rm E}$$
 $V_{\rm E}$ V_{\rm

PAGE 1-B

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-

oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)-, ethyl ester (9CI)

MF C34 H37 N O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-acetyl-2-[2-(5-methyl-2-phenyl-4-

oxazolyl)ethoxy]phenyl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]- (9CI)

MF C38 H34 F N O6

F

$$CO_2H$$
 $O-CH-CH_2-CH_2-CH=CH$
 $CH_2-CH_2-CH_2-O$

Ph

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-6-[5-methoxy-2-[[4-

(trifluoromethyl)phenyl]methoxy]phenyl]- (9CI)

MF C28 H27 F3 O6

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 8-Dodecenoic acid, 12-(4-hydroxy-3-methoxyphenyl)-10-oxo-, ethyl ester
(9CI)

MF C21 H30 O5

$$CH_2-CH_2-CH=CH-(CH_2)_6-C-OEH$$

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester (9CI)

MF C16 H20 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-(5-fluoro-2-hydroxyphenyl)-2-[4-

(trifluoromethyl)phenoxy]- (9CI)

MF C19 H16 F4 O4

L8 REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-1-oxo-1H-inden-5-yl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-(9CI)

MF C38 H32 F N O6

$$\begin{array}{c} \text{Me} \\ \text{O} \\ \text{Ph} \\ \text{O} \\ \text{CH}_2 - \text{O} \\ \text{O} \\ \text{CH}_2 - \text{CH} \\ \text{CH}_2 - \text{CH} \\ \text{CH}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2006 ACS on STN L8 91 ANSWERS

5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[(5-IN methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-, ethyl ester (9CI)

MF C38 H36 F N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester (9CI)
MF C20 H28 O3

$$CH_2-CH_2-C \equiv C-(CH_2)_3-C-OMe$$
 $O-(CH_2)_4-Me$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Hexenoic acid, 6-[[2-(2,2-dibromoethenyl)phenyl]amino]-,
 1,1-dimethylethyl ester, (2E)- (9CI)
MF C18 H23 Br2 N O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN α-D-Glucopyranoside, methyl 4,6-O-[(R)-phenylmethylene]-,
 bis(9-phenyl-4,6-nonadiynoate) (9CI)
MF C44 H42 O8

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 2-(4-benzo[b]thien-2-ylphenoxy)-6-phenyl- (9CI)
MF C26 H22 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C31 H27 F4 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C31 H28 F3 N O6

F3C
$$CO_2H$$
 $O-CH-CH_2-CH_2-CH=CH$ CH_2-O CH_2-O CH_2-O CH_2-O CH_2-O CH_2-O CH_2-O CH_2-O

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C27 H36 O5 S

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C21 H21 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)

MF C28 H24 F6 O5

MeO
$$CH = CH - CH_2 - CH_2 - CH - O$$
 CF_3 CF_3 CF_3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-phenyl-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester
(9CI)

MF C21 H21 F3 O3

$$\begin{array}{c} \begin{array}{c} \\ \\ \\ \text{Eto-C} \\ \\ \\ \text{Ph-CH} \end{array} = \text{CH-CH}_2 - \text{CH}_2 - \text{CH-O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS. REGISTRY COPYRIGHT 2006 ACS on STN

IN 7-Dodecenoic acid, 12-(3,4-dimethoxyphenyl)-10-hydroxy-9-[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI)

MF C29 H40 O7 S

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C16 H22 O5

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY, COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-(2-hydroxy-5-methylphenyl)-2-(2-methoxyphenoxy)- (9CI)

MF C20 H22 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-1-oxo-1H-inden-5-yl]-2-(2-methoxyphenoxy)-, ethyl ester (9CI)

MF C35 H35 N O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)

MF C32 H30 F3 N O6

F3C
$$CO_2H$$
 $O-CH-CH_2-CH_2-CH=CH$ CH_2-CH_2-O CH_2-CH_2-O OMe O

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-, ethyl ester (9CI)

MF C35 H32 F4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Hexenoic acid, 6-[[2-(2,2-dibromoethenyl)-4-(phenylmethoxy)phenyl]amino], 1,1-dimethylethyl ester, (2E)- (9CI)

MF C25 H29 Br2 N O3

Double bond geometry as shown.

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN α -D-Glucopyranoside, methyl 4,6-O-[(R)-phenylmethylene]-, 2-(9-phenyl-4,6-nonadiynoate) (9CI)

MF C29 H30 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-(4-benzo[b]thien-3-ylphenoxy)-6-phenyl- (9CI)

MF C26 H22 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)

MF C32 H33 N O7

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-(2-methoxyphenoxy)- (9CI)
MF C20 H22 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 8-Dodecenoic acid, 10-oxo-12-phenyl-, ethyl ester (9CI) MF C20 H28 O3.

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN INDEX NAME NOT YET ASSIGNED MF C22 H23 N O4

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2-[(2-fluorophenyl)methoxy]-5-methoxyphenyl]-2-[4(trifluoromethyl)phenoxy]- (9CI)

MF C27 H24 F4 O5

MeO
$$CH = CH - CH_2 - CH_2 - CH_0$$
 CF_3 CF_3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-fluorophenyl]-2-[4-

(trifluoromethyl)phenoxy]- (9CI)

MF C28 H27 F4 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-phenyl-2-[4-(trifluoromethyl)phenoxy]- (9CI)

MF C19 H17 F3 O3

$$CO_{2H}$$
 $Ph-CH=CH-CH_{2}-CH_{2}-CH-O$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 8-Dodecenoic acid, 12-(3,4-dimethoxyphenyl)-10-oxo-, ethyl ester (9CI)

MF C22 H32 O5

$$\begin{array}{c|c} O & O & O \\ \parallel & \parallel \\ CH_2-CH_2-C-CH \end{array}$$

$$\begin{array}{c|c} CH_2-CH_2-C+CH \end{array}$$

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Heptenoic acid, 4,5-dihydroxy-7-(4-methoxyphenoxy)-, ethyl ester,

(2E, 4R, 5R) - (9CI)

MF C16 H22 O6

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Heptenoic acid, 6-oxo-7-phenyl-, ethyl ester (9CI)

MF C15 H18 O3

$$\begin{array}{c|c} \mathsf{O} & \mathsf{O} & \mathsf{O} \\ \parallel & \parallel & \parallel \\ \mathsf{Ph}-\mathsf{CH}_2-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH} & \mathsf{CH}-\mathsf{C}-\mathsf{OEt} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]1-oxo-1H-inden-5-yl]-2-(2-methoxyphenoxy)- (9CI)

MF C33 H31 N O7

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[2-[(2-fluorophenyl)methogyl 5-methogyl 605)

fluorophenyl)methoxy]-5-methoxyphenyl]- (9CI)

MF C32 H28 F2 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-, ethyl ester
(9CI)

MF C20 H21 F O3

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \end{array} \\ \text{Eto-C} \\ \\ \\ \text{H}_2\text{C} = \text{CH-CH}_2 - \text{CH}_2 - \text{CH-O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C20 H25 Br2 N O4

Double bond geometry as shown.

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)

MF C30 H28 F6 O5

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[2-[(2-fluorophenyl)methoxy]-5-methoxyphenyl]-2-(2-methoxyphenoxy)- (9CI)

MF C27 H27 F O6

MeO
$$CH = CH - CH_2 - CH_2 - CH_0$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-, ethyl ester (9CI)

MF C15 H20 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 8-Dodecenoic acid, 10-oxo-12-phenyl- (9CI)
MF C18 H24 O3

$$^{\rm O}_{||}$$
 Ph-CH₂-CH₂-C-CH=CH-(CH₂)6-CO₂H

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN Tetradecanoic acid, 2-([1,1'-biphenyl]-2-yloxy)- (9CI) MF C26 H36 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-(2-hydroxy-5-methoxyphenyl)-, ethyl ester (9CI)

MF C27 H27 F O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-methoxy-2-[(5-methyl-2-phenyl-4oxazolyl)methoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)

MF C31 H31 N O7

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[4-(5-chloro-2-thienyl)phenoxy]-6-phenyl-, ethyl ester
(9CI)

MF C24 H23 C1 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 7-Dodecenoic acid, 10-hydroxy-9-[[(4-methylphenyl)sulfonyl]oxy]-12-phenyl, ethyl ester (9CI)

MF C27 H36 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF (C99 H168 N6 O8)n

RELATED POLYMERS AVAILABLE WITH POLYLINK

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Heptenoic acid, 6-hydroperoxy-6-methoxy-7-phenyl-, ethyl ester (9CI)

MF C16 H22 O5

REGISTRY COPYRIGHT 2006 ACS on STN L8 91 ANSWERS

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-phenyl-, ethyl ester (9CI)

MF C26 H25 F O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2006 ACS on STN L8 91 ANSWERS

IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-methoxyphenyl]-2-

(2-methoxyphenoxy) - (9CI)

MF C29 H33 N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2006 ACS on STN L8

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[[4-

(trifluoromethyl)phenyl]methoxy]phenyl]- (9CI)

MF C33 H28 F4 O5

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Heptenoic acid, 7-[[2-(2,2-dibromoethenyl)phenyl]amino]-,
1,1-dimethylethyl ester, (2E)- (9CI)
MF C19 H25 Br2 N O2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN IN 4,6-Nonadiynoic acid, 9-phenyl- (9CI)

MF C15 H14 O2

 $HO_2C-CH_2-CH_2-C \equiv C-CH_2-CH_2-Ph$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-, ethyl ester (9CI)

MF C39 H38 F N O6

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)
MF C31 H30 F N O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-(2-methoxyphenoxy)-,
 ethyl ester (9CI)
MF C22 H26 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 7-Dodecenoic acid, 10-hydroxy-12-[3-methoxy-4-(methoxymethoxy)phenyl]-9[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI)
MF C30 H42 O8 S

=> e 2-Heptenoic acid, 5-hydroxy-7-(4-methoxyphenoxy)-, ethyl ester,/cn

ALL ANSWERS HAVE BEEN SCANNED

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

```
2-HEPTENOIC ACID, 5-HYDROXY-7-((4-METHOXYPHENYL)METHOXY)-4-M
                   ETHYL-, METHYL ESTER, (2E, 4S, 5R)-/CN
E2
                   2-HEPTENOIC ACID, 5-HYDROXY-7-((4-METHOXYPHENYL)METHOXY)-4-M
                   ETHYL-, METHYL ESTER, (R-(R^*,S^*-(E)))-/CN
E3
             0 --> 2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL EST
                   ER,/CN
E4
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL EST
                   ER, (2E, 5S) - /CN
E5
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, ETHYL ESTER,
                    (E) - /CN
             1
Е6
                   2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, METHYL ESTER
                    (2E, 5R) - /CN
E7
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, METHYL ESTER
                   (S-(E))-/CN
E8
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-METHOXY-5-METHYL-, ETHYL ESTER
                   /CN
E9
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, Δ-LACTONE/CN
E10
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, ETHYL ESTER, (2E)-/CN
E11
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, ETHYL ESTER, (2E,5S)-
                   /CN
E12
             1
                   2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, METHYL ESTER, (2E)-/C
=> e4
             1 "2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL ESTER,
Ь9
                (2E, 5S) - "/CN
=> d 19
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN
     912457-38-6 REGISTRY
ED
     Entered STN: 06 Nov 2006
CN
     2-Heptenoic acid, 5-hydroxy-7-(4-methoxyphenoxy)-, ethyl ester,
     (2E,5S)- (9CI) (CA INDEX NAME)
FS
     STEREOSEARCH
MF
     C16 H22 O5
SR
     CA
LC
     STN Files:
                  CA, CAPLUS
```

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

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SINCE FILE ENTRY SESSION 190.24

TOTAL

190.45

FULL ESTIMATED COST

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=> 19

L10 1 L9

=> d l10 ti fbib abs

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

- TТ De Novo Asymmetric Synthesis of Milbemycin β3 via an Iterative Asymmetric Hydration Approach
- 2006:784680 CAPLUS AN
- DN 145:418819
- TI De Novo Asymmetric Synthesis of Milbemycin $\beta 3$ via an Iterative Asymmetric Hydration Approach
- Li, Miaosheng; O'Doherty, George A.
- CS Department of Chemistry, West Virginia University, Morgantown, WV, 26506, USA
- SO Organic Letters (2006), 8(18), 3987-3990 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- דת Journal
- LA English

AB The enantioselective synthesis of the spiroketal/macrolide natural product milbemycin $\beta 3$ (I) has been achieved in 22 steps and 2.8% overall yield from an achiral dienoate. The spiroketal ring system was installed by three sequential asym. hydrations followed by sprioketalization. Both the absolute and relative stereochem. of milbemycin $\beta 3$ was introduced by two Sharpless asym. dihydroxylations, two π -allylpalladium-catalyzed redns., and an iridium-catalyzed hydrogen migration/Claisen rearrangement to install the C-12 stereocenter.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> e 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester/cn
 REG1stRY INITIATED
Substance data EXPAND from CAS REGISTRY in progress...

Ι

| E1 | 1 | 5-OCTYNOIC ACID, 7-((1R, 3AS, 4E, 7AR)-4-((2Z)-((3S, 5R)-3, 5-BIS (((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-2-METHYLENECYCLOHEXY |
|-----|-----|--|
| | | LIDENE) ETHYLIDENE) OCTAHYDRO-7A-METHYL-1H-INDEN-1-YL) -4-HYDRO |
| | • | XY-2-METHYLENE-, MET/CN |
| E2 | 1 | 5-OCTYNOIC ACID, 8,8'-(2,2-DIMETHYL-1,3-DIOXOLANE-4,5-DIYL)B |
| | | IS(8-(BENZOYLOXY)-, DIMETHYL ESTER, (4R-(4A(R*),5.BETA.(R*)))-/CN |
| E3 | ۸ ۰ | |
| | | 5-OCTYNOIC ACID, 8-2-(PENTYLOXY) PHENYL -, METHYL ESTER/CN |
| E4 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-2 |
| | | ,2-DIMETHYL-8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER/CN |
| E5 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8 |
| | | -(2-(PENTYLOXY)-3-PYRIDINYL)-, METHYL ESTER/CN |
| E6 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8 |
| | | -(2-(PENTYLOXY)PHENYL)-, METHYL ESTER/CN |
| E7 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8 |
| | | -(2-(PENTYLOXY)PHENYL)-, METHYL ESTER, (8R)-/CN |
| E8 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8 |
| | | -(2-(PENTYLOXY)PHENYL)-, METHYL ESTER, (8S)-/CN |
| E9 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8 |
| | | -(3-(PENTYLOXY)-2-NAPHTHALENYL)-, METHYL ESTER/CN |
| E10 | 1 | 5-OCTYNOIC ACID, 8-((3AR, 5S, 6AR)-TETRAHYDRO-2,2-DIMETHYLFURO |
| | _ | (2,3-D)-1,3-DIOXOL-5-YL)-8-(((TRIFLUOROMETHYL)SULFONYL)OXY)- |
| | | /~/~ ~/ T/~ DIOVOT-0-IT)-0-(((IKILTOOKOMETUIT))DOTLONIT)OKI)- |

| | | , METHYL ESTER, (8R)-/CN |
|-----|---|--|
| E11 | 1 | 5-OCTYNOIC ACID, 8-((4S,6R)-2,2-DIMETHYL-6-((1E)-3-OXO-1-PRO |
| | | PENYL)-1,3-DIOXAN-4-YL)-8-IODO-, METHYL ESTER, (8S)-/CN |
| E12 | 1 | 5-OCTYNOIC ACID, 8-((4S,6R)-2,2-DIMETHYL-6-(1E)-1,3-NONADIEN |
| | | YL-1.3-DIOXAN-4-YL)-8-IODO-, METHYL ESTER, (8S)-/CN |

| => file reg | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.46 | 199.61 |
| | | |
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| | ENTRY | SESSION |
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=> e 5-Octynoic acid, 8-(2-(pentyloxy)phenyl)-, methyl ester/.cn '.CN' IS NOT VALID HERE
The user-defined search field specified does not exist. For more information, enter HELP SET FIELD at an arrow prompt (=>).

```
=> e 5-Octynoic acid, 8-(2-(pentyloxy)phenyl)-, methyl ester/cn
E1
             1
                   5-OCTYNOIC ACID, 8-((4S,6R)-6-(BIS(ETHYLTHIO)METHYL)-2,2-DIM
                   ETHYL-1,3-DIOXAN-4-YL)-8-IODO-, METHYL ESTER, (8S)-/CN
E2
                   5-OCTYNOIC ACID, 8-((4S,6R)-6-FORMYL-2,2-DIMETHYL-1,3-DIOXAN
                   -4-YL) -8-IODO-, METHYL ESTER, (8S)-/CN
             1 --> 5-OCTYNOIC ACID, 8-(2-(PENTYLOXY) PHENYL)-, METHYL ESTER/CN
E3
                   5-OCTYNOIC ACID, 8-(2-FURANYL)-8-HYDROXY-, METHYL ESTER/CN
E4
                   5-OCTYNOIC ACID, 8-(2-FURANYL)-8-METHOXY-/CN
E.5
             1
                   5-OCTYNOIC ACID, 8-(2-FURANYL)-8-METHOXY-, METHYL ESTER/CN
E6
             1
                   5-OCTYNOIC ACID, 8-(2-OXABICYCLO(3.1.0) HEX-3-EN-6-YL)-8-OXO-
E7
             1
                   , METHYL ESTER/CN
E8
             1
                   5-OCTYNOIC ACID, 8-(3-FURANYL)-, METHYL ESTER/CN
E9
                   5-OCTYNOIC ACID, 8-(6-(1-(ACETYLOXY)-4,4-DIMETHOXY-2-NITRONO
                   NYL) -2, 2-DIMETHYL-1, 3-DIOXAN-4-YL) -8-METHOXY-, METHYL ESTER,
                    (4S-(4A(S^*),6A(1R^*,2S^*)))-/CN
E10
             1
                   5-OCTYNOIC ACID, 8-(6-(1-(ACETYLOXY)-4,4-DIMETHOXY-2-NITRONO
                   NYL) -2, 2-DIMETHYL-1, 3-DIOXAN-4-YL) -8-METHOXY-, METHYL ESTER,
```

(4S-(4A(S*),6B(1S*,2R*)))-/CN

5-OCTYNOIC ACID, 8-(6-(1-HYDROXY-4,4-DIMETHOXY-2-NITRONONYL)
-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER, (4S
-(4A(S*),6B(1R*,2S*)))-/CN

E12

1 5-OCTYNOIC ACID, 8-(6-(1-HYDROXY-4,4-DIMETHOXY-2-NITRONONYL)
-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER, (4S
-(4A(S*),6B(1S*,2R*)))-/CN

=> e3

1 "5-OCTYNOIC ACID, 8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER"/CN

=> d 111

L11

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 898909-76-7 REGISTRY

ED Entered STN: 06 Aug 2006

CN 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)

MF C20 H28 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

$$CH_2-CH_2-C \equiv C-(CH_2)_3-C-OMe$$
 $O-(CH_2)_4-Me$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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| | | ECEN-1-YNYL)-5-OXOCYCLOPENTYL)-, METHYL ESTER, (1R-(1A |
|-----|----|---|
| | | ,2B(3S*,5S*),3A))-/CN |
| E2 | 1 | 2-HEPTYNOIC ACID, 7-(4,7-DIHYDRO-5,7-DIOXO-5H-THIENO(2,3-C)P |
| | | YRAN-4-YL)-, METHYL ESTER/CN |
| E3 | 1> | 2-HEPTYNOIC ACID, 7-(4-METHOXYPHENOXY)-, ETHYL ESTER/CN |
| E4 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((3-METHYL-4-(3-THIE |
| | | NYLMETHYL) PHENYL) AMINO) -6-QUINAZOLINYL ESTER/CN |
| E5 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-(2-THIENYLMETHOX |
| | | Y) PHENYL) AMINO) -6-QUINAZOLINYL ESTER/CN |
| E6 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-(PHENYLMETHOXY))P |
| | | HENYL) AMINO) -6-QUINAZOLINYL ESTER/CN |
| E7 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-PHENOXYPHENYL)AM |
| | | INO)-6-QUINAZOLINYL ESTER/CN |
| E8 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-(6-CHLORO-2,3-DIHYDR |
| | | O-1H-INDOL-1-YL)-6-QUINAZOLINYL ESTER/CN |
| E9 | 1 | 2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-(6-CHLORO-7-FLUORO-2 |
| | | ,3-DIHYDRO-1H-INDOL-1-YL)-6-QUINAZOLINYL ESTER/CN |
| E10 | 1 | 2-HEPTYNOIC ACID, 7-(4-PROPYL-2,6,7-TRIOXABICYCLO(2.2.2)OCT- |
| • | | 1-YL)-, METHYL ESTER/CN |
| E11 | | 2-HEPTYNOIC ACID, 7-(4-PYRIDYL)-/CN |
| E12 | 1 | 2-HEPTYNOIC ACID, 7-(4-PYRIDYL)-, HYDROCHLORIDE/CN |
| | | |

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=> e3 L13 1 "2-HEPTYNOIC ACID, 7-(4-METHOXYPHENOXY)-, ETHYL ESTER"/CN => d 113

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

FILE COVERS 1907 - 1 Dec 2006 VOL 145 ISS 23 FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> 111

L12 1 L11

=> d l12 ti fbib abs

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI Synthesis of aromatic analogs of 8(S)-HETE and their biological evaluation as activators of the PPAR nuclear receptors

AN 2006:477347 CAPLUS

DN 145:145433

TI Synthesis of aromatic analogs of 8(S)-HETE and their biological evaluation as activators of the PPAR nuclear receptors

AU Caijo, Frederic; Mosset, Paul; Gree, Rene; Audinot-Bouchez, Valerie; Boutin, Jean; Renard, Pierre; Caignard, Daniel-Henri; Dacquet, Catherine

CS Laboratoire de Syntheses et Activations de Biomolecules, CNRS UMR 6052, ENSCR, Beaulieu, 35700, Fr.

SO European Journal of Organic Chemistry (2006), (9), 2181-2196 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

OS CASREACT 145:145433

GΙ

$$R^1$$
 $X-Y$
 CO_2Na
 R^2
 W
 O
 Me
 I

AB A new family of 8-HETE analogs, such as I [R1 = R2 = H, W = CH2, X-Y = (CH2)2, C.tplbond.C, CH:CH-(Z); R1 = R2 = H, W = N, X-Y = (CH2)2-, C.tplbond.C, CH:CH-(Z); R1R2 = CH:CHCH:CH, W = CH2, X-Y = (CH2)2, C.tplbond.C, CH:CH-(Z)], were synthesized as dual PPAR α and PPAR γ agonists. A versatile strategy was developed to allow modulations not only around the aromatic core but also on the side chains of these analogs. The affinity of these compds. towards the PPAR α and PPAR γ receptors was reported, together with their transactivation percentage. The derivs. having a propargylic type side chain gave the most promising results as dual agonists.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> e 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester/cn
 REG1stRY INITIATED
Substance data EXPAND from CAS REGISTRY in progress...

RN 912457-36-4 REGISTRY

ED Entered STN: 06 Nov 2006

CN 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester (9CI) (CA

INDEX NAME)

MF C16 H20 O4

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> 113

L14 1 L13

=> d l14 ti fbib abs

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI De Novo Asymmetric Synthesis of Milbemycin $\beta 3$ via an Iterative Asymmetric Hydration Approach

AN 2006:784680 CAPLUS

DN 145:418819

TI De Novo Asymmetric Synthesis of Milbemycin $\beta 3$ via an Iterative Asymmetric Hydration Approach

AU Li, Miaosheng; O'Doherty, George A.

CS Department of Chemistry, West Virginia University, Morgantown, WV, 26506, USA

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PB American Chemical Society

DT Journal

LA English

GI

The enantioselective synthesis of the spiroketal/macrolide natural product milbemycin $\beta 3$ (I) has been achieved in 22 steps and 2.8% overall yield from an achiral dienoate. The spiroketal ring system was installed by three sequential asym. hydrations followed by sprioketalization. Both the absolute and relative stereochem. of milbemycin $\beta 3$ was introduced by two Sharpless asym. dihydroxylations, two π -allylpalladium-catalyzed redns., and an iridium-catalyzed hydrogen migration/Claisen rearrangement to install the C-12 stereocenter.

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```
=> e 6-phenyl-2,4-hexadienoic acid/cn
E1
                                          6-PHENYL-2,4-HEPTANEDIONE/CN
                             1
E2
                             1
                                           6-PHENYL-2,4-HEXADIENE/CN
E3
                             0 --> 6-PHENYL-2,4-HEXADIENOIC ACID/CN
E4
                             1
                                          6-PHENYL-2,4-HEXANEDIONE/CN
E5
                             1
                                           6-PHENYL-2,4-LUTIDINE/CN
E6
                             1
                                           6-PHENYL-2, 4-PYRIMIDINEDIAMINE/CN
E7
                             1
                                           6-PHENYL-2-((2-PROPYNYL)OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL)
                                           OXY) PHENYL) ETHYL) HEXANAMIDE/CN
E8
                             1
                                           6-PHENYL-2-(2-TOLYL)-2,3,4,5-TETRAHYDROPYRIDAZIN-3-ONE/CN
E9
                                           6-PHENYL-2-(3-PHENYLPROPYL) HEXANOIC ACID/CN
                             1
E10
                             1 .
                                           6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-P
                                           YRIMIDIN-4-ONE/CN
E11
                             1
                                           6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-P
                                           YRIMIDIN-4-ONE HYDROCHLORIDE/CN
E12
                             1
                                           6-PHENYL-2-(PYRIDIN-4-YL)PYRIMIDIN-4-OL/CN
=> 5-phenoxy-2,4-pentadienoic acid/cn
                             0 5-PHENOXY-2,4-PENTADIENOIC ACID/CN
=> e e1
E1
                             1
                                           6-PHENYL-2,4-DIOXOPERHYDRO-1,3,5-TRIAZINE/CN
E2
                             1
                                           6-PHENYL-2, 4-DIOXOPYRAN/CN
                             1 --> 6-PHENYL-2,4-HEPTANEDIONE/CN
E3
F.4
                             1
                                           6-PHENYL-2,4-HEXADIENE/CN
E5
                             1
                                           6-PHENYL-2,4-HEXANEDIONE/CN
                                           6-PHENYL-2,4-LUTIDINE/CN
E6
                             1
E7
                             1
                                           6-PHENYL-2, 4-PYRIMIDINEDIAMINE/CN
                             1
E8
                                           6-PHENYL-2-((2-PROPYNYL)OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((3-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((3-PROPYNYL))OXY)-N-(2-(3-METHOXY-4-((3-PROPYNYL))OXY)-N-(3-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOX-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOX-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY-4-(3-METHOXY
                                           OXY) PHENYL) ETHYL) HEXANAMIDE/CN
E9
                             1
                                           6-PHENYL-2-(2-TOLYL)-2,3,4,5-TETRAHYDROPYRIDAZIN-3-ONE/CN
E10
                             1
                                           6-PHENYL-2-(3-PHENYLPROPYL) HEXANOIC ACID/CN
E11
                             1
                                           6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-P
                                           YRIMIDIN-4-ONE/CN
E12
                                           6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-P
                                           YRIMIDIN-4-ONE HYDROCHLORIDE/CN
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